

Original Article: A comparison between density functional theory calculations and the additive schemes of polarizabilities of the Li-F-decorated BN cages



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ABSTRACT

Density functional calculations are performed to investigate the polarizabilities of the LiF decorated $B_{12}N_{12}$ cages ($B_{12}N_{12}Li_nF_n$ derivatives, $n=1-12$). The mean polarizability of LiF decorated $B_{12}N_{12}$ cages ($23.455-238.882 \text{ \AA}^3$) is higher than that of $B_{12}N_{12}$ (20.831 \AA^3). DFT calculations have shown that polarizabilities of LiF decorated $B_{12}N_{12}$ cages marginally depend on the position and the number of decorated LiF units. Polarizabilities of $B_{12}N_{12}Li_nF_n$ cages grow linearly with the increase of the number of LiF units decorated. We also use depression of polarizability to characterize the polarizabilities of these cages. A linear relation is found between the polarizability and the number of added units, which could be significant in the design of decorated BN cages with polar characteristics.

Introduction

The electric polarizability of the molecule can be understood as the degree to which the electron cloud of the molecule fills the space. It is a useful quantity in suggesting the electric and magnetic properties of a compound [1].

Polarizability, for example, makes it possible to clarify the characteristics of molecular interactions in molecular systems [2, 3], to estimate their reactivity in reactions [4], and to evaluate the dipole moments of molecules [5]. Polarizability is also known as a significant physical property in evaluating the potential applications of complexes in nanotechnology [6]. Fowler and colleagues [7] and Pederson and Kuong [8] theoretically

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studied, for the time, polarizabilities of fullerene cages. The direct measurement of polarizabilities of the fullerene cages showed the high polarizability of fullerene cages so that the polarizability of these systems cannot be ignored when analyzing their physical and chemical behaviors [10-14]. Then, many theoretical studies were conducted on the polarizabilities of fullerene derivatives [9-11]. Although some theoretical studies on the fullerene cages have been carried out [11-16], as far as we know, no theoretical calculations on boron-nitride cages, have been published.

Boron nitride nanostructures are known as cousins of carbon nanostructures due to their heteropolar properties; they show different interesting properties, such as higher thermal stability and conductivity, and low dielectric constant, being higher antioxidant [17-24]. For example, due to their large surface area, BN cages have received great attention in the field of hydrogen storage [25-28]. Among them, it can be proved theoretically that the magic $B_{12}N_{12}$ cage is a material suitable for storing hydrogen [29]. On the other hand, lithium-decorated BN cages show charge transfer from Li to the BN cage, resulting in point charges and polarization which lead to an electric field and binding of hydrogens [31-33]. As of these cages, polarized hydrogen molecules are bound with decorated Li atoms in a quasi-molecular form, in which binding energies are found to be between physical and chemical adsorption. So, the adsorbed hydrogen will be desorbed under ambient conditions. For example, it is predicted that $Li_{12}C_{60}$ can reversibly accumulate up to 13% of hydrogen in the quasi-molecular form [29].

Previously, Anafcheh et al. [35] theoretically studied the effect of silicon doping on the stability and electronic structures of fullerenes and then tried to calculate the diagonalized polarizability tensors through density functional theory in order to find mean polarizability and anisotropy of polarizability for some silicon fullerene derivatives. So, it would be a good idea for us to investigate mean polarizability in the present study for series of $B_{12}N_{12}$ cages with different coverage of host lithium fluoride through density functional

theory calculations and additive schemes which offer valuable information for their future experimental detections and can facilitate their application in various fields such as sensors or hydrogen storage.

Although some studies have been conducted on the polarizability of fullerene derivatives, there is no theoretical calculation to investigate the simultaneous existence Li and F atoms on the polarizability of the boron-nitride cages [2-4].

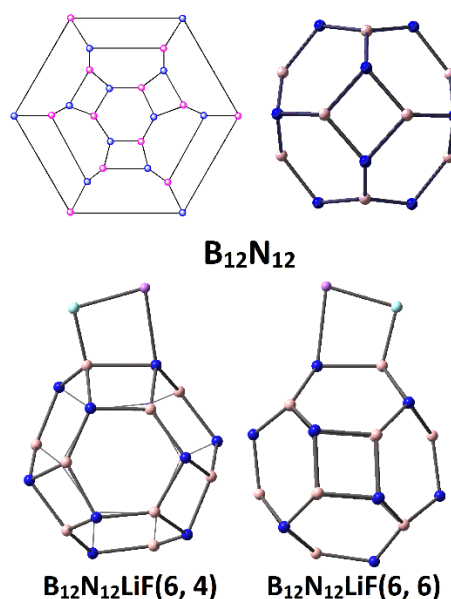


Figure 1. The Schlegel diagram and the optimized structure of $B_{12}N_{12}$ together with the optimized structures of the LiF-decorated $B_{12}N_{12}$ cages, $B_{12}N_{12}LiF(6, 4)$ and $B_{12}N_{12}LiF(6, 6)$

Computational Methods

Structures of LiF-decorated $B_{12}N_{12}$ derivatives are fully optimized at the computational level of M06-2X/6-311+G(d, p) [36, 37]. This level is accurate enough for fullerene derivatives [38, 39]. Frequency calculations are calculated for all the systems on the same computational level, which yield real frequencies approving that they are all structures with the minimum energy. All the results are obtained using the GAMESS software package for calculations [40, 41]. The other properties are computed on the

optimized structures. Using the finite-field approach, we computed tensor components of polarizability as the second-order derivatives of the total energy with respect to the homogenous external electric field F :

$$\alpha_{ij} = - \left(\frac{\partial^2 E}{\partial F_i \partial F_j} \right) \quad (1)$$

The tensor of polarizability is diagonalized as follows, calculated in any coordinate system. The accuracy of the procedure of diagonalization was confirmed by the trace invariants of the tensor of the coordinate system:

$$\text{tr } \alpha = \text{tr } \alpha_{diag} \quad (2)$$

The average polarizability of the system is calculated using α_{xx} , α_{yy} and α_{zz} , the eigenvalues of the polarizability tensors:

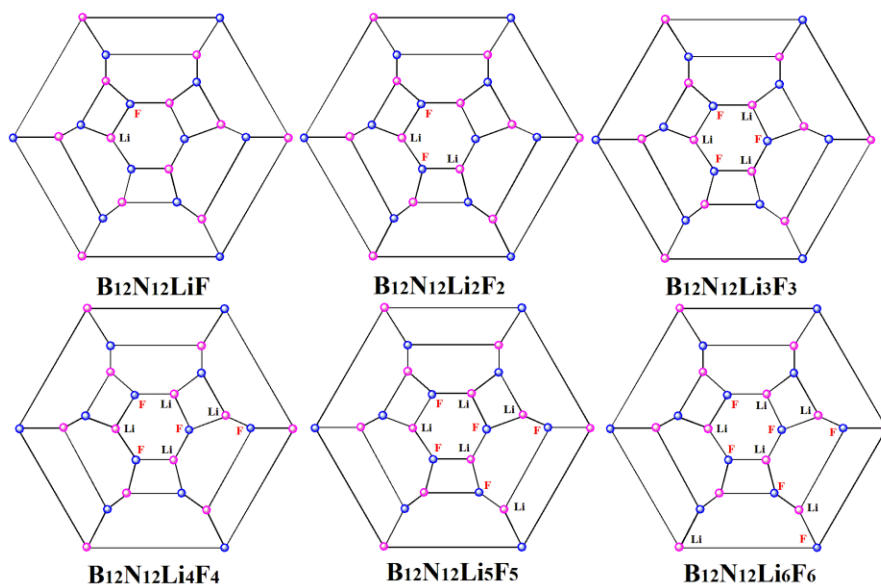
$$\alpha = \frac{1}{3} (\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad (3)$$

Results and Discussion

$B_{12}N_{12}$ consists of 8 hexagons and 6 squares, which meet the isolated square rule (ISR) to the maximal separation of the strained square rings. As shown in Fig.1, square rings correspond to the vertices of the octahedral

structure. The optimized $B_{12}N_{12}$ cage consists of two nonequivalent B-N bonds namely bonds on the junction of a square and a hexagon ring (S-H bonds) and bonds on the junction of a hexagon and a hexagon ring (H-H bonds). The S-H bond lengths are obtained to be 1.511 Å which are longer than those of H-H bonds (1.441 Å). It should be noted that both are shorter than the length of single BN bonds (1.668 Å) and longer than the double BN bonds at the same level of theory.

$B_{12}N_{12}$ cage is decorated with LiF at the S-H or H-H junction, and the resulted LiF-decorated $B_{12}N_{12}$ is indicated by $B_{12}N_{12}LiF(6, 4)$ and $B_{12}N_{12}LiF(6, 6)$ respectively (see Fig. 1). According to our results, the α values of LiF decorated $B_{12}N_{12}$ cages are obtained to be higher than that of $B_{12}N_{12}$ (20.831 Å³). On the other hand, the mean polarizability of the $B_{12}N_{12}LiF(6, 4)$ in which LiF units decorated on the S-H junction of $B_{12}N_{12}$ (23.455 Å³), is almost equal to those of and $B_{12}N_{12}LiF(6, 6)$ in which LiF units are decorated on the LiF on an H-H junction (23.473 Å³). Therefore, the results indicate polarizabilities of isomers which are almost independent of the position of LiF units but mainly depend on their numbers.



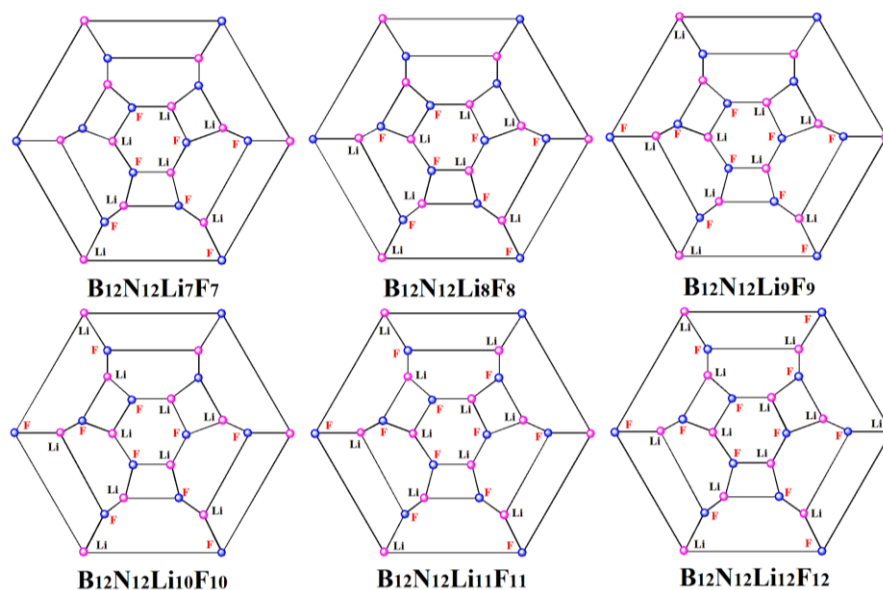


Figure 2. The Schlegel diagrams of the LiF-decorated $B_{12}N_{12}$ cages

Table 1. The calculated values of α , α_{add} , and α_{corr} of the LiF-decorated $B_{12}N_{12}$ cages ($B_{12}N_{12}Li_nF_n$, $n=1-12$)

	α	α_{add}	$\Delta\alpha$	$\Delta\alpha/n$	$\Delta\alpha/n-1$	α_{corr}
$B_{12}N_{12}LiF$	23.473	23.694	0.221			23.473
$B_{12}N_{12}Li_2F_2$	24.987	26.558	1.571	0.786	2.469	24.632
$B_{12}N_{12}Li_3F_3$	26.483	29.421	2.939	0.980	2.159	25.791
$B_{12}N_{12}Li_4F_4$	27.460	32.285	4.825	1.206	2.586	26.950
$B_{12}N_{12}Li_5F_5$	28.371	35.148	6.777	1.355	2.870	28.109
$B_{12}N_{12}Li_6F_6$	31.216	38.011	6.795	1.133	1.847	29.268
$B_{12}N_{12}Li_7F_7$	31.135	40.875	9.740	1.391	2.635	30.427
$B_{12}N_{12}Li_8F_8$	32.667	43.738	11.071	1.384	2.501	31.586
$B_{12}N_{12}Li_9F_9$	35.868	46.602	10.734	1.193	1.800	32.745
$B_{12}N_{12}Li_{10}F_{10}$	34.423	49.465	15.042	1.504	2.794	33.904
$B_{12}N_{12}Li_{11}F_{11}$	38.102	52.329	14.226	1.293	2.024	35.063
$B_{12}N_{12}Li_{12}F_{12}$	38.882	55.192	16.310	1.359	2.199	36.222

For clarity, the decoration pattern is illustrated with Schlegel diagrams in Figure 2. The LiF decoration takes into account “hexagon filling”, and “continuity” rules. The LiF decoration on the hexagon-hexagon BN bond in the cage of $B_{12}N_{12}$ results in $B_{12}N_{12}LiF$. Then, further LiF decoration in the same hexagon, until its saturation, leads to $B_{12}N_{12}Li_3F_3$. After saturation of one hexagon, LiF decoration continues in one direction, such that the other hexagons are covered one by one until the formation of $B_{12}N_{12}Li_{12}F_{12}$. Figure 2 depicts $B_{12}N_{12}Li_{12}F_{12}$ in which twelve hexagon-hexagon BN bonds are decorated. The calculated

polarizability values of $B_{12}N_{12}Li_nF_n$ derivatives ($n=1$ to 12) are shown in Table 1. The α value of $B_{12}N_{12}Li_nF_n$ derivatives ($n=1$ to 12) are found to be higher than that of $B_{12}N_{12}$, and the mean polarizability of the $B_{12}N_{12}Li_nF_n$ derivatives ($n=1$ to 12) increases by increasing LiF units, reaching the maximum value of 38.882 in $B_{12}N_{12}Li_{12}F_{12}$. This should be noted when designing highly polarized materials.

Although there are several quantum chemical methods for calculating polarizability, it is still relevant to evaluate it in terms of additive schemes. Therefore, in order to study

the relationship between polarizability and molecular structure and the interaction between molecular fragments, it is important to compare the quantum quantities obtained with additives. Since Le Fèvre [42] developed the first additive polarization scheme, two trends of improvement schemes have been developed: (1) When determining the addition scheme, consider the correlation between the polarizability parameter of the atom and the bond of the closest molecular fragment types [43]. The first type is applied in this work; and (2) developing an additive scheme, and describe any deviation from it as a manifestation of the interaction between atoms.

Sabirov *et al.* [16] successfully used the additive scheme for epoxide fullerene derivatives, indicating that the increase for fullerene epoxides corresponds to the addition of oxygens to the cage, while for silicon epoxides, it is related to the substitution of each oxygen for a pair of hydrogen atoms. Based on this scheme, the $B_{12}N_{12}Li_nF_n$ ($n+1$) is considered as the subunits of $B_{12}N_{12}$ cage and n decorated LiF units. The mean polarizability of the subunits is estimated at the same level of theory:

$$\alpha_{\text{add}}(B_{12}N_{12}Li_nF_n) = \alpha(B_{12}N_{12}) + n\alpha_0 \quad (4)$$

Where $\alpha_0 = \alpha(B_{12}N_{12}LiF) - \alpha(B_{12}N_{12}) = 2.642 \text{ \AA}^3$. The α and α_{add} values are calculated for the $B_{12}N_{12}Li_nF_n$ cages with n up to 12 (Table 2).

As seen in Figure 3, polarizability parameters of $B_{12}N_{12}Li_nF_n$ rise linearly (α and

α_{add}) if $n \rightarrow 12$, and also their differences increase with the increase of n .

Depression of polarizability, $\Delta\alpha$, is a common parameter studied for exohedrally decorated fullerene derivatives, whose magnitude varies for different structures [16].

We calculate the depression of polarizability ($\Delta\alpha$) and the negative derivation of $\alpha_{\text{add}}(B_{12}N_{12}Li_nF_n)$ from $\alpha(B_{12}N_{12}Li_nF_n)$, as follows:

$$\Delta\alpha = \alpha_{\text{add}}(B_{12}N_{12}Li_nF_n) - \alpha(B_{12}N_{12}Li_nF_n) \quad (5)$$

The polarizability depression can be used to study the reciprocal influence of the core and LiF units decorated. According to the equation obtained from $\Delta\alpha = 1.4719 n - 1.2133$ ($R^2 = 0.9794$), the increase in the polarizability depression as n decreases corresponds to the linear correlation between n and $\Delta\alpha$. When the deviation parameter $\Delta\alpha$ is proportional to the polarizability depression of the totally decorated $B_{12}N_{12}Li_{12}F_{12}$ cage, it could be obtained as follows:

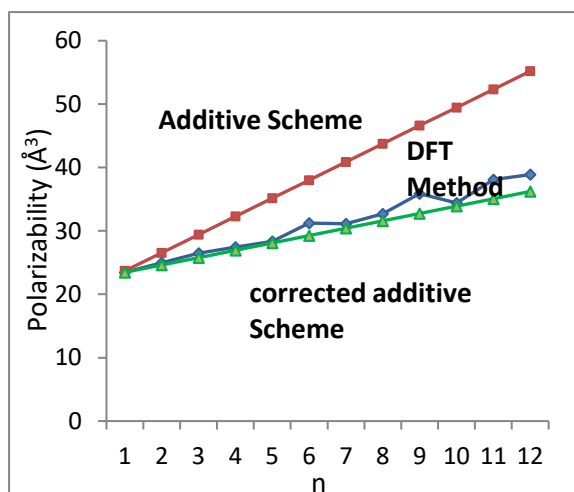
$$\Delta\alpha(B_{12}N_{12}Li_nF_n) \sim \Delta\alpha(B_{12}N_{12}Li_{12}F_{12}) \quad (6)$$

Increasing the polarizability depression linearly with n implies that:

$$\Delta\alpha(B_{12}N_{12}Li_nF_n) \sim n \quad (7)$$

In fact, $\Delta\alpha(B_{12}N_{12}Li_nF_n)/(n-1)$ is almost independent of n (especially for $n > 1$), so we have:

$$\Delta\alpha(B_{12}N_{12}Li_nF_n) \sim (n-1)\Delta\alpha(B_{12}N_{12}Li_{12}F_{12}) \quad (8)$$



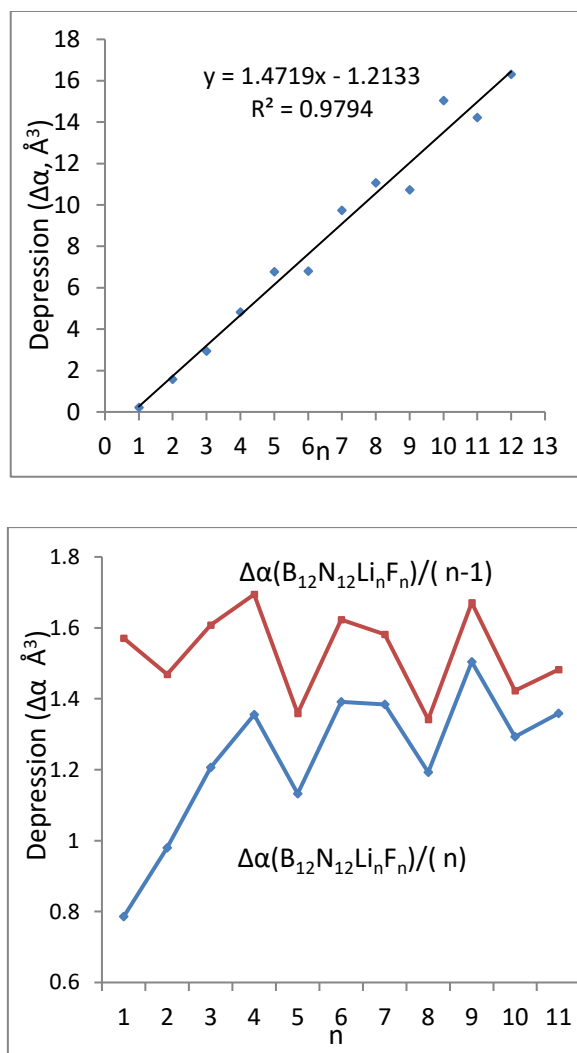


Figure 3. Dependences of polarizability on number of LiF units using DFT method and additive scheme

By introducing the coefficient of k , the relation of (8) results in the equation as follows:

$$\Delta\alpha(B_{12}N_{12}Li_nF_n) = k(n - 1)\Delta\alpha(B_{12}N_{12}Li_{12}F_{12}) \quad (9)$$

When $n = n_{max}$, Eq. (9) is true if $k = \frac{1}{n_{max}-1}$

$$\Delta\alpha(B_{12}N_{12}Li_nF_n) = \frac{(n-1)\Delta\alpha(B_{12}N_{12}Li_{12}F_{12})}{n_{max}-1} \quad (10)$$

With appropriate accuracy, Eq. 13 describes $\Delta\alpha(B_{12}N_{12}Li_nF_n)$ for all the values of n (Fig. 3). It covers the variations in the polarisability upon the interaction of moieties of the $B_{12}N_{12}Li_nF_n$ complexes. Sabirov et al. [44] presented a similar formula for fullerene halogenides $C_{60}X_n$.

It is possible to use Eq. 14 as an improvement to the additive scheme. Finally, mean polarizabilities $\alpha(B_{12}N_{12}Li_nF_n)$ can be calculated in terms of the corrected additive scheme:

$$\alpha(B_{12}N_{12}Li_nF_n) = \alpha(B_{12}N_{12}) + N\alpha_0 - \frac{(n-1)\Delta\alpha(B_{12}N_{12}Li_{12}F_{12})}{n_{max}-1} \quad (11)$$

Parameters of Eq. 14 are shown in Table 2. The fitting function is found to be:

$$\alpha_{corr}(DFT) = 20831 + 1.159n = 1.483 \quad (12)$$

The fitting function renders the quantum-chemically values of the $B_{12}N_{12}Li_nF_n$ polarisabilities with high accuracy (Figure 3).

Conclusion

Density functional theory computations were performed to investigate the polarizabilities of LiF-decorated derivatives of $B_{12}N_{12}$ ($B_{12}N_{12}Li_nF_n$ ($n=1-12$) derivatives). It is found that the mean polarizabilities, α , of the LiF decorated $B_{12}N_{12}$ cages are obtained to be higher than that of $B_{12}N_{12}$. Our DFT calculations on LiF decorated $B_{12}N_{12}$ cages show that polarizabilities of isomers are almost independent of the position of LiF units while mainly depend on their numbers. For $B_{12}N_{12}Li_nF_n$ ($n=1-12$), mean polarizabilities linearly increase with the increase of the number of LiF units and are related to the negative depression of polarizability. The formula used to relate the polarizability to the number of added groups could be applied in material science, valuable in the design of BN cage derivatives with regulated polar characteristics.

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No potential conflict of interest was reported by the authors.

Conflict of interest

The authors declare no conflicts of interest.

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