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A computational study of adsorption of hydrogen and diatomic molecules on azadibenzo-corannulene

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***Abstract*— In this work, adsorption energies of molecular hydrogen and diatomic molecules (Li_2, F_2 and Cl_2) on azadibenzo-corannulene have been studied by density functional theory calculations. Our DFT results using the B97-3c functional show that the azadibenzo-corannulene with a nitrogen on the rim can enhance the adsorption energy of diatomic molecules on the surface.**

***Keywords*— Azadibenzo-corrannulene, DFT, adsorption, van der Waals interaction, gas storage**

I. Introduction

During the last decades, a considerable attention has been devoted to the discovery of new materials with high adsorption capacity to capture and store gases such as metal-organic frameworks and graphene-based materials. Among newly synthetised polycyclic aromatic hydrocarbons, the bowl-shaped corannulene in which nitrogen atom was incorporated on the rim has been reported by Tsefrikas et al.[1] (Fig. 1).

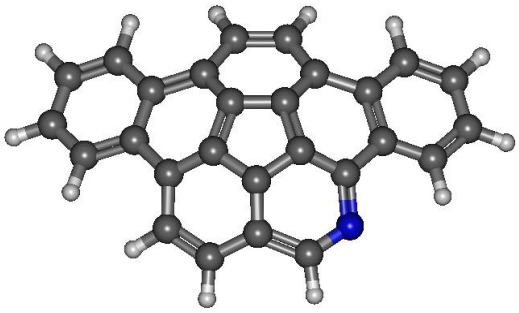

Fig. 1 Molecular structure of 5-Azadibenzo[a,g]corannulene

There have been a number of theoretical studies of gas molecular adsorption on nitrogen-doped polycyclic aromatic hydrocarbons [2,3].

II. Computational Methods

We performed computational investigation based on the study of interaction of diatomic molecules with 5-Azadibenzo[a,g]corannulene by using the recently developed composite method B97-3c [4] implemented in ORCA 4.0 [5], the results are visualised with graphical interface software GABEDIT [6].

We first define the adsorption energy of diatomic molecule on 5-Azadibenzo[a,g]corannulene. The value of the adsorption energy noted E_{ads} is calculated by using the following equation:

$$E_{ads} = E_{Azadibenzocorannulene\text{-}diatomic} - (E_{Azadibenzocorannulene} + E_{diatomic})$$

Where E_{ads} is the adsorption energy of diatomic molecule on the azadibenzo-corannulene after optimization, $E_{Azadibenzo\text{-}corannulene\text{-}diatomic}$ represents the electronic energy of the Azadibenzo-corannulene system with diatomic molecule, $E_{Azadibenzocorannulene}$ and $E_{diatomic}$ are the total energies of Azadibenzocorannulene and the diatomic molecules in an isolated form.

The interaction of the gas molecules with the 5-Azadibenzo[a,g]corannulene has been studied by performing calculations for the configuration where the axis of the molecules are in perpendicular orientation to the plane of 5-Azadibenzo[a,g]corannulene. The molecules were initially put about 3Å from the azadibenzo-corannulene in the middle over the basal plane and in the vicinity of the edge over the N atom.

III. Results and Discussion

The results of the calculated adsorption energies are summarized in table 1.

TABLE 1
Calculated Adsorption Energies (E_{ads})

Diatomic molecules	**H_2**	**Li_2**	**F_2**	**Cl_2**
E_{ads} (Kj/mol) On the edge (over the N atom)	-7.35	-86.08	-17.87	-48.60
E_{ads} (Kj/mol) On the middle (over the five carbon ring)	-6.79	-48.65	-17.56	-24.96

As shwon in table 1, the interaction between diatomic molecules and 5-Azadibenzo[a,g]corannulene is enhanced by

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the presence of nitrogen on the rim, particularly for Li_2 and Cl_2. For Li_2 and Cl_2, the short intermolecular contacts of 1.99 Å and 2.38 Å between nitrogen of 5-Azadibenzo[a,g]corannulene and nearest Lithium or chlorine atoms of diatomic molecules is indicative of weak intermolecular forces and pointing to an attractive interaction resulting in an increased adsorption energy (Fig. 2)

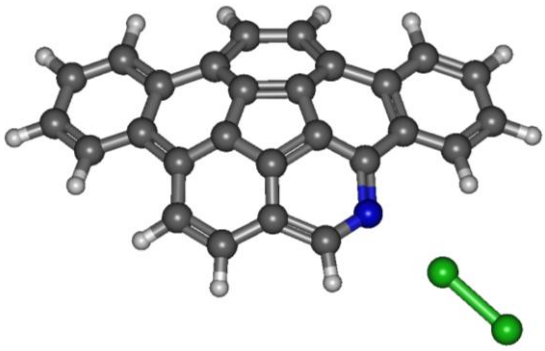

Fig. 2 Interaction of $Cl_2$with the 5-Azadibenzo[a,g]corannulene

The bond length of the adsorbed Li_2, F_2 and Cl_2 are 3.19 Å, 1.57 Å and 2.16 Å respectively, longer than that of isolated molecules 2.67 Å, 1.45 Å and 1.99 Å, indicating that adsorption process weakened the original X-X bond of diatomic molecules.

IV. Conclusions

The adsorption of diatomic molecules Li_2, H_2, F_2 and Cl_2 on 5-Azadibenzo[a,g]corannulene was investigated by means of DFT calculations using B97-3c functional. Our results predict a Stronger adsorption process between Li_2 and Cl_2 and 5-Azadibenzo[a,g]corannulene in the vicinity of nitrogen atom with adsorption energies of -86.08 kJ/mol and -48.60 kJ/mol respectively.

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