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# Density functional study of cyanogen ($C_2N_2$) sensing using OH functionalized fullerene (C60) and germanium-fullerene (Ge60)

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ABSTRACT

Behavior of $C_2N_2$ adsorption on the surface of C60 and Ge60 was investigated by density functional theory calculation. The effects of OH functionalization on the adsorption of $C_2N_2$ gas via C60 and Ge60 surfaces were investigated. Results reveal that C60 and Ge60 were the most favorable cases toward the $C_2N_2$ adsorption, energetically. Results show that, $E_{ad}$ value of $C_2N_2$ on Ge60 surface were more negative than corresponding values of C60. Results reveal that, OH functionalization increase the absolute $E_{ad}$ values of $C_2N_2$ on studied fullerenes. These results show that, there are linearity dependencies between $E_{ad}$ and orbital energy values of studied fullerenes.



## 1. Introduction

Cyanogen ($C_2N_2$) is created by the oxidation of hydrogen cyanide and it is very toxic [1,2]. Cyanogen is an irritant to the eyes and respiratory system [3,4]. The study of adsorption of toxic gas on the solid surface of nanostructure materials are important in environmental issue [5–8]. The carbon fullerene (C60) is important nanoscale material and it has high performance in science and technology [9–13].

The germanium-fullerene (Ge60) is not experimentally available but it is a benchmark model system with important future prospects, particularly in the adsorption of toxic gases. In previous study the structures and electronic states of alkyl-radical-functionalized C20 fullerenes have been investigated by density functional theory (DFT) and also different alkyl radicals investigated were methyl, and butyl radicals [14]. Gallo and et al. [15] used DFT calculations to study the effects of covalently binding isoniazid, an antitubercular compound to functionalized carbon nanotubes and fullerenes. Anafcheh and et al. [16] used computational study to investigation the cyclo sulfurization of the pentagon–pentagon junctions in the fullerenes C60.

Gueorguiev and et al. [17] utilized first-principles calculations to study the formation mechanisms of the fullerene-like structure in carbon nitride compounds in the context of aligned incorporation of CN precursors along edges of evolving sheets during vapor phase synthesis. They used the B3LYP hybrid functional because it is produce an accurate description of the structural and electronic properties of similar systems such as the novel aza-fullerene [17].

Furlan and et al. [18] studied nanostructured CPx compounds by first principles calculations. Their results obtained by B3LYP hybrid functional which it is known to provide an accurate description of the structural and electronic properties of fullerene-like thin films and similar covalent systems [18]. Their results show that Geometry optimizations and cohesive energy comparisons show stability for $C_3P$, $C_2P$, $C_3P_2$, CP, and $P_4$ ($P_2$) species in isolated form as well as incorporated in graphene layers [18].

In the present work, the interactions of $C_2N_2$ gas with C60, Ge60 and their OH functionalized structures investigated, this study can show the potential of C60 and Ge60 as sensor of $C_2N_2$.

## 2. Computational details

In this study, structure of C60, Ge60 and their OH functionalized derivatives and structures of complexes of studied fullerenes with $C_2N_2$ were geometry optimized (structures were shown in Fig. 1). All the calculations were performed using the DFT/B3LYP method and 6-311G(d) basis set within the GAMESS package [19,20]. The B3LYP is a commonly used approach in topics related with the investigations of studied fullerenes [21–25].

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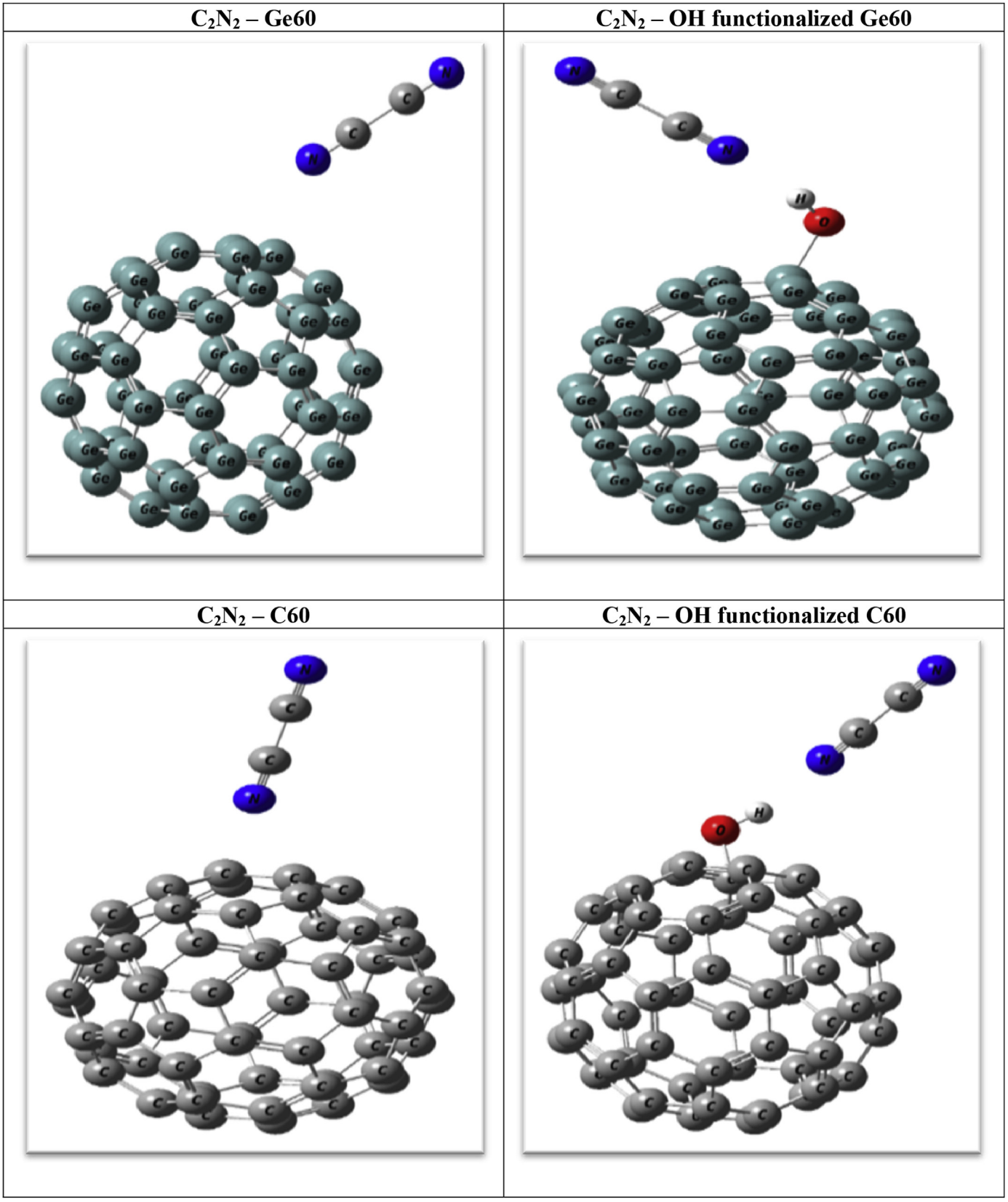


**Fig. 1.** Structure of complexes of $C_2N_2$ with studied nanostructures.