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**Original Research Article**

# Fullerene ($C_{24}$) as a Potential Sensor for the Detection of Acrylamide: A DFT Study

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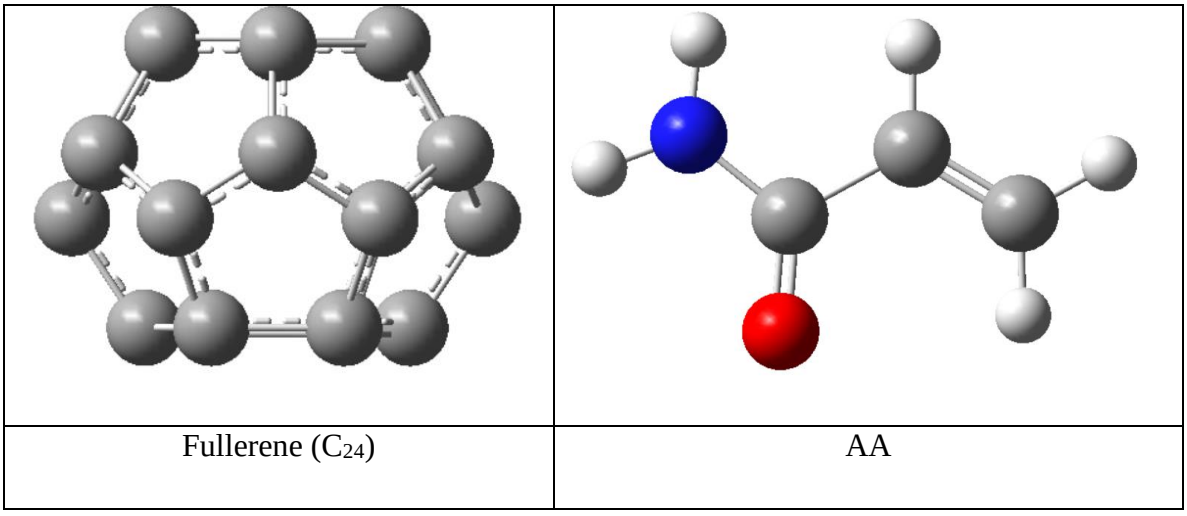
**ABSTRACT**

Acrylamide is a toxic chemical that is formed in starchy foods like potato chips and can cause cancer in humans. Therefore, its detection is of great importance. In this research, the performance of $C_{24}$ fullerene as an electrocatalytic sensing material for acrylamide was checked out by DFT simulations. The obtained adsorption energies showed acrylamide interaction with $C_{24}$ is experimentally feasible. The calculated thermodynamic parameters including $\Delta G_{ad}$, $\Delta H_{ad}$, and $K_{th}$ showed acrylamide adsorption process is spontaneous, exothermic, and reversible. The NBO results demonstrated no chemical bond has created between acrylamide and fullerene in the adsorption procedure, hence the adsorption nature is a physisorption. The calculated frontier molecular orbital indices showed the bandgap of fullerene experienced a -52% decline after interacting with acrylamide. Therefore, this nanostructure can be employed as an excellent electrocatalytic sensing material for the fabrication of a new electrochemical sensor for the determination of acrylamide.

**Keywords: Acrylamide, Density functional theory, Adsorption, Fullerene ($C_{24}$), Sensor**

## Introduction

Acrylamide (AA, Figure 1) is an organic compound with the chemical formula $CH_2$=CHC(O)$NH_2$. It is a white odorless solid, soluble in water and several organic solvents [1-3]. AA was discovered in foods, mainly in starchy foods, such as potato chips, French fries, and bread that had been heated higher than 120 °C (248 °F) [4-7]. Production of AA in the heating process was shown to be temperature-dependent. It was not found in food that had been boiled, or in foods that were not heated [8-10]. AA can arise in some cooked foods via a series of steps by the reaction of the amino acid asparagine and glucose. This condensation, one of the Maillard reactions, followed by dehydrogenation produces N-(D-glucos-1-yl)-L-asparagine, which upon pyrolysis generates some acrylamide [11-13]. The main toxicity risks of AA are neurotoxicity, adverse effects on male reproduction, developmental toxicity and carcinogenicity. Therefore, development of a rapid, sensitive and accurate analytical method for AA is of great importance. Electrochemical sensors are portable analytical devices that have simple and economic instrumentation, high selectivity and sensitivity, time-saving analysis procedure, and applicability in opaque and colored samples [14-16]. Hence, electrochemical sensors can be an ideal device for the measurement of AA. On the other hand, the first and main step in the development of a new electrochemical sensor for the detection of an analyte is finding an appropriate material that has a good and selective interaction with the desired compound. $C_{24}$ (Figure 1) is one of the smallest fullerenes with $D_6$ symmetry that consists of two hexagonal and twelve pentagonal rings [17].



| Fullerene ($C_{24}$) | AA |
|---|---|

**Figure 1.** Optimized structures of AA and $C_{24}$

This nanostructure has high chemical and structural stability, excellent electrical conductivity, and great specific surface area [17]. These traits make $C_{24}$ an ideal candidate for research in molecule electronic devices, biomedical engineering, and nanotechnology [17]. Therefore, this research was focused on examining the performance of fullerene ($C_{24}$) as a sensing material for the detection of AA using density functional theory computations.

## COMPUTATIONAL METHODS

Software versions GuassView 6 [17] and Nanotube modeler 1.3.0.3 [18] were used to design the structures of $C_{24}$, AA, and their complexes [19]. Each of the structures that were designed first underwent geometric optimization. After that, computations for infra-red (IR), frontier molecular orbital (FMO), and natural bond orbital (NBO) were performed on designed structures. The density functional theory (DFT) method was used throughout the computations by Gaussian 16 [39] software at the B3LYP/6-31G (d) level of theory [20]. This level was selected since the findings obtained from earlier studies were acceptable and were consistent with experimental results. All computations were performed in the vacuum and aqueous phases.

The following processes were investigated [20]:

Adsorbate + Adsorbent → Drug-Adsorbent 1

Adsorption energy values ($E_{ad}$) and thermodynamic parameters, such as thermodynamic equilibrium constant ($K_{th}$), Gibbs free energy changes ($\Delta G_{ad}$), and adsorption enthalpy changes ($\Delta H_{ad}$), entropy changes ($\Delta S_{ad}$) were calculated using equations 2–6.

$$E_{ad} = \left(E_{(Adsorbate-Adsorbent)} - \left(E_{(Adsorbate)} + E_{(Adsorbent)}\right)\right) + EBSSE \quad (2)$$

$$\Delta H_{ad} = \left(H_{(Adsorbate-Adsorbent)} - \left(H_{(Adsorbate)} + H_{(Adsorbent)}\right)\right) \quad (3)$$

$$\Delta G_{ad} = \left(G_{(Adsorbate-Adsorbent)} - \left(G_{(Adsorbate)} + G_{(Adsorbent)}\right)\right) \quad (4)$$

$$\Delta S_{ad} = \left(S_{(Adsorbate-Adsorbent)} - \left(S_{(Adsorbate)} + S_{(Adsorbent)}\right)\right) \quad (5)$$

$$K_{th} = \exp\left(-\frac{\Delta G_{ad}}{RT}\right) \quad (6)$$

In the equations above, E stands for the total electronic energy for every structure, $E_{BSSE}$ stands for the basis set superposition correction, and H represents the total energy of the evaluated materials plus the thermal correction of enthalpy. For each structure under study, the G denotes

the total energy plus the thermal correction of the Gibbs free energy [42]. R represents the constant of the ideal gas, S is the thermal correction entropy for the studied structures, and T stands for temperature [20].

Equations 8 and 9 were used to calculate the bandgap ($E_g$), variations of nanostructure bandgap ($\%\Delta E_g$) [20].

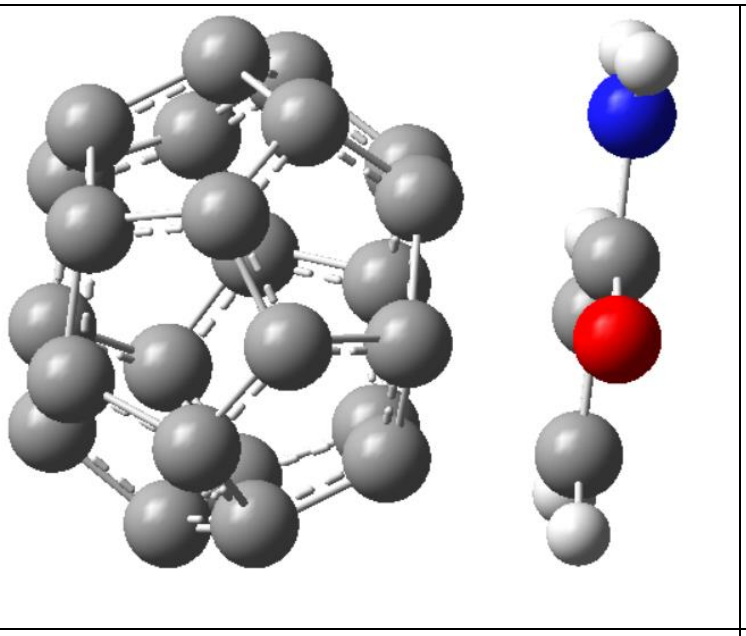
$$E_g = E_{LUMO} - E_{HOMO} \quad (7)$$

$$\%\Delta E_g = \frac{E_{g2} - E_{g1}}{Eg1} \times 100 \quad (8)$$

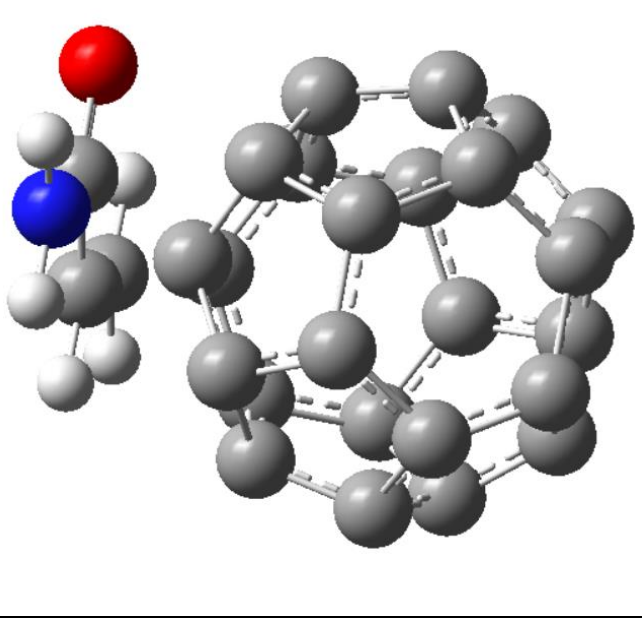
$E_{LUMO}$, in the equations above, is the energy of the lowest unoccupied molecular orbital, and $E_{HOMO}$ is the energy of the highest occupied molecular orbital. The bandgaps of the Nano-adsorbent and AA-Adsorbent complexes are shown as $E_{g1}$ and $E_{g2}$, respectively [20].

## Results and Discussion

In order to find the most stable configuration, the adsorption phenomenon was scrutinized at two different conformers (Figure 2). In A-conformer, the AA molecule was inserted in a parallel form towards the hexagonal ring of fullerene. But, in B-conformer, the AA molecule was inserted in a parallel form towards the pentagonal ring of fullerene.



**A-Conformer**



**B-Conformer**

**Figure 2.** Optimized structures of AA complexes with $C_{24}$

As the provided optimized structures in figure 2 shows clearly, no tangible deformation has occurred in the structures of adsorbent and adsorbate in both conformers indicating the adsorption is a physisorption. The calculated values of adsorption energies, $\Delta H_{ad}$, $\Delta G_{ad}$, $\Delta S_{ad}$ and $K_{th}$ are given in Table 1. As can be seen, all values are negative implying the interaction is experimentally possible, spontaneous, exothermic, and inappropriate in terms of entropy. The effect of solvent was also checked out and the obtained results showed the presence of solvent cannot affect the system meaningfully.

For acquiring more information about interactions nature NBO computations were also carried out on the structures and the results showed no covalent bond has created between AA and fullerene. Therefore, interaction nature is a physisorption. The FMO parameters of the structures were also calculated and the obtained results are given in Table 2. As it is clear, the bandgap of fullerene experienced a %26 increment after adsorption of AA indicating the electrochemical conductance of nanostructure has declined during the adsorption process and this phenomenon can be used as an analytical signal in the detection of AA. Hence, fullerene could be used as a novel sensing material for the development of a novel electrochemical sensor for the determination of AA.

**Table 1.** The calculated values of adsorption energy, $\Delta H_{ad}$, $\Delta G_{ad}$, $\Delta S_{ad}$, $K_{th}$, $\nu_{min}$ in vacuum and aqueous phases

| NO | Adsorption energy (kJ/mol) | $\Delta G_{ad}$ (kJ/mol) | $\Delta H_{ad}$ (kJ/mol) | $\Delta S_{ad}$ (J/mol.K) | $K_{th}$ | $\nu_{min}$ ($cm^{-1}$) |
|---|---|---|---|---|---|---|
| **A-Conformer (Vacuum)** | -196.091 | -83.015 | -49.128 | -22.55 | $1\times10^{-12}$ | 14.220 |
| **A-Conformer (Water)** | -102.008 | -64.829 | -38.432 | -14.76 | $1\times10^{-8}$ | 13.170 |
| **B-Conformer (Vacuum)** | -177.615 | -73.477 | -42.880 | -31.76 | $1\times10^{-9}$ | 7.260 |
| **B-Conformer (Water)** | -106.001 | -50.921 | -32.670 | -22.781 | $1\times10^{-7}$ | 8.140 |

**Table 2.** The calculated FMO parameters

| NO | $E_{HOMO}$ (eV) | $E_{LUMO}$ (eV) | $E_g$ (eV) | $\%\Delta E_g$ |
|---|---|---|---|---|
| **AA** | -2.740 | 2.730 | 4.470 | --- |
| **$C_{24}$** | -4.380 | 1.380 | 5.760 | --- |
| **A-Conformer** | -3.220 | 4.041 | 7.261 | 26.059 |
| **B-Conformer** | -3.888 | 3.612 | 7.300 | 26.736 |

## Conclusion

In this research, the function of $C_{24}$ as a sensing material for the detection of AA was evaluated by DFT computations. The results exhibited $C_{24}$ interaction with AA is experimentally feasible, spontaneous, and exothermic. The influence of solvent was also investigated and the achieved results showed the presence of water as the solvent does not affect the interactions. On the other hand, the FMO calculations showed the electrical conductivity of fullerene decreased remarkably after adsorption of AA. Hence, this nanostructure can be used as an electrocatalytic modifier for the development of a new electrochemical sensor for the determination of AA.

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