[FUNTIONALIZED *FULLERENES CAGES (C59M) AS PROMISSING MATERIALS FOR CAPTURING ENVIRONMENTA POLLUTIONS CO2, NO2 AND SO2 GASES]*

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Overview

Energy is necessary to the continuation of life on Earth. Using energy allows us to live, travel and move as well as to light up the dark and feel fine during the winter and the summer. Most of this energy generated from fossil fuels. Using fossil fuels excessively has placed the world in front of one of the biggest problems of the era, and this has led to pollution of the Earth's atmosphere. The increasing demand for energy globally and the rapid technological progress, cause both the amount of fuel needed to generate electricity and the amount of greenhouse gases and other air pollution emitted are increased as a result.

Clean air is what all living humans and animals need for good health. However, due to unstoppable urban development, the air is continuously polluted. Urban ambient air is more polluted than the overall atmosphere due to the high density of the human population and their activities in urban areas. The atmosphere, or air, is normally composed of 79-percent nitrogen, 20-percent oxygen, and one percent mixture of carbon dioxide, water vapor, and small quantities of several other gases. When the fossil fuels are burned, the combustion gases include the emission of carbon dioxide (CO_2), sulphur dioxide (SO_2), nitrogen oxide (NO_x) and other polluted gases. Nearly all combustion products have negative effects on the environment and human health. Where, the CO_2 contributes to the greenhouse effect. Although, the SO_2 exists in small concentrations in the earth's atmosphere, it causes acid rain, and it is found in the case of volcanic eruptions and the effluents released from industries. Nitrogen oxides (NO_x) is a highly poisonous gas knowing as Nitrogen dioxide and it is one of the major atmospheric pollutants that absorb UV light and stops to reach it to the earth's surface.

The emissions caused by electricity generation vary due to many factors, including the amount of electricity is generated, the electricity generation technologies used, and the air pollution control devices used. It is difficult to control the first two factors, however the third factor needs more research to obtain promising materials to build a new devices for capturing the air pollutions to improve the air quality and hence the human health.

Therefore, this work will use the functionalized fullerene cages C59M (M=Li, He, Be, B, N, F, Al and Ti) with elements from eight different groups to select the most candidate fullerene cages to use as pollutions control through adsorption the polluted gases and captured them.

Methods

All calculations are performed with DFT as implemented within G09W package, using B3LYP exchange-functional and applying 6-311G++(d,2p) basis set. All structures are fully optimized without any constraint. The DFT technique was used owing to the accuracy associated and confirmed in many previous work [1-12]. The electronic properties, including the density of states (DOSs), HOMO (highest occupied orbital), LUMO (lowest unoccupied orbital), Energy gaps E_g, E_{FL} (Energy of Fermi level, and natural bond orbital (NBO) charge analysis are calculated. Also, the adsorption energies (Eads) are obtained from the following equation,

$$E_{ads} = E_{C59M-gas} - (E_{C59M} + E_{gas})$$

where $E_{C59M-gas}$ is the energy of the optimized C_{59}M-gas structure, E_{C59M} is the energy of the optimized C_{59}M structure and E_{gas} is the energy of polluted gas. The energy gap between HOMO and LUMO (Eg) was well-defined as $E_g = E_{LUMO} - E_{HOMO}$ whereas E_{LUMO} and E_{HOMO} are energy of HOMO and LUMO.

The energy of Fermi level (E_{FL}) that lies in the middle of the HOMO and LUMO

$$E_{FL} = \frac{E_{LUMO} + E_{HOMO}}{2}$$

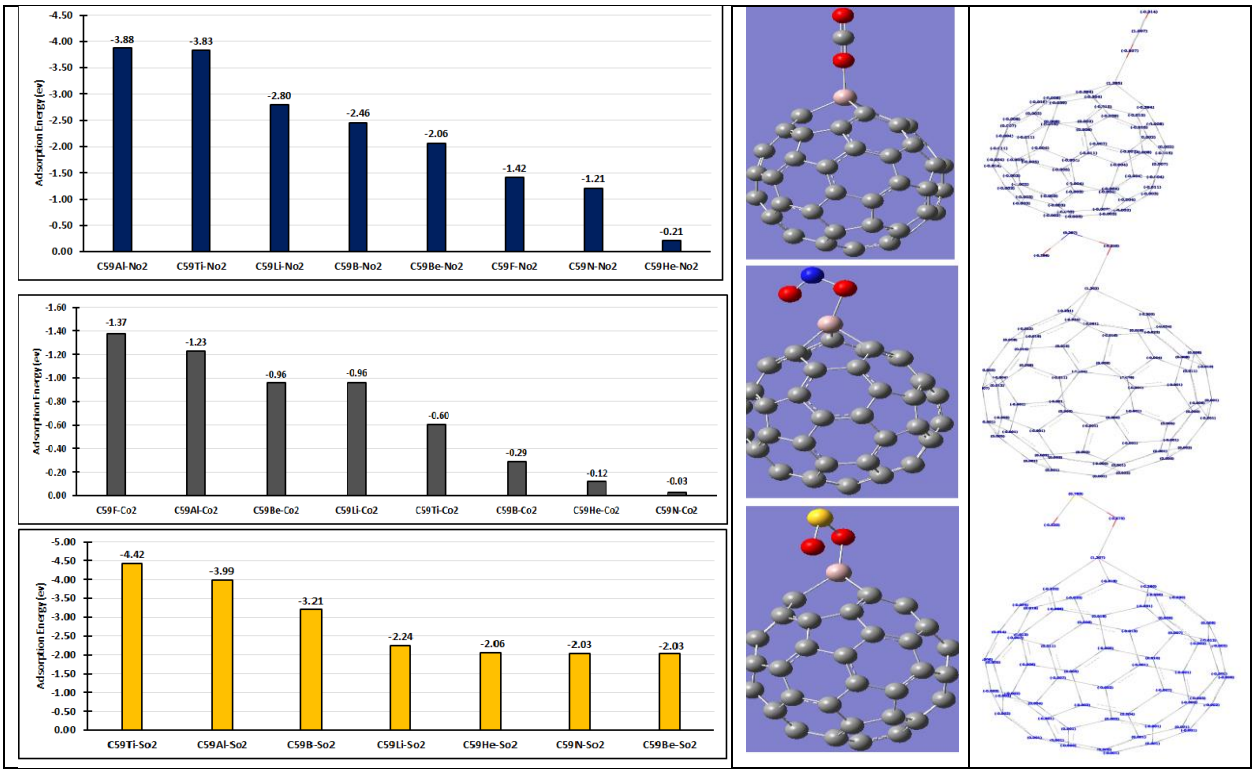
The enthalpy change (ΔH) and Gibbs free energy change (ΔG) will be calculated at T=298 K and P = 1 atm as

$$\Delta H = E_{C59M-gas} - (H_{C59M} + H_{gas})$$

$$\Delta G = G_{59M-gas} - (G_{C59M} + G_{gas})$$

where H(G)C_{59}M-gas, H(G)C_{59}M, and H(G)gas are the sum of electronic and thermal enthalpies (the sum of electronic and thermal free energies) of C_{59}M-gas, C_{59}M cages, and gas molecule, respectively.

Results



This work includes 24 fully optimized structures of adsorbed polluted gases (CO_2, NO_2 and SO_2) on functionalized fullerene cages C59M (M=Li, He, Be, B, N, F, Al and Ti) with elements from eight different groups (alkali metals, Nobel gas, Alkaline earth metal, Metalloids, non-metals, halogen, post transition metal and transition metals), respectively. The above Figure shows the adsorption energies of polluted gases are negative reflecting the powerful of functionalized fullerene cages C59M for capturing the polluted gases. Also, the natural bond orbital charge analysis and optimized structures for C59Al-CO_2, C59Al-NO_2 and C59Al-SO_2 are shown as example for polluted gases captured through functionalised fullerene cage by Aluminium.

Conclusions

Using the Density Functional Theory and applying the G09W program, the fully optimized structures, the dipole moments, the density of states, the band gaps including the HOMO and LUMO are obtained. Also, the natural bond orbital, enthalpy change, and Gibbs free energy change are studied. The results show that the functionalization of fullerene cages increases their activities to capture the polluted gases and the best functionalized fullerenes cages for capturing the polluted gases are C59Ti and C59AL.

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