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Hydrogen Adsorption on Beryllium-C_{60} Fullerene: a Theoretical Study

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ABSTRACT

Nowadays chemists have focused their efforts in the design and preparation of new materials capable of storing gases responsible for the greenhouse effect, such as CO, CO_2, N_2O, SO_2. Also, there is great interest in the design of materials capable of storing H_2 molecules due to their potential application as an alternative energy source for hydrocarbons. These efforts are complemented by theoretical studies using, computational chemistry. Based on the above, we have explored the potential energy surface of $[C_{60}]$-Be_n complexes to find how many beryllium atoms can interact with the fullerene. Results with the B3LYP/def2-TZVP method suggest that fullerene can accommodate up to 20 beryllium atoms on its surface. Complexes of the type $[C_{60}]$-Be_nH_{2n} (n = 1-20) also were calculated at the same level of theory, in order to find the maximum number of hydrogen molecules coordinated to each beryllium atom. Results show that metallic atoms are η^2 bonded on the fullerene surface. On the other hand, beryllium atoms can coordinate up to two hydrogen molecules with two-electron three-center bonds. Be-H and H-H bond lengths have values from 1.45-1.51 and 0.81-0.85 Å, respectively. The availability of those complexes, for hydrogen storage, will be discussed in more detail during the congress of hydrogen.

Keywords: fullerene, beryllium, DFT