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Interaction between the Li and planes (100) of FULLERITES of the form $[C60]_5$, $[C70]_5$, $[C80]_5$ e $[C96]_5$, with analysis of the HOMO-LUMO, charges, distances, dipoles, using MNDO, HF and DFT methods

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Abstract – We studied the interaction of the lithium atoms with (100) planes of fullerites of the form $[C60]_5$, $[C70]_5$, $[C80]_5$ and $[C96]_5$. We observed a reduction of the energy gap (HOMO-LUMO) of the system as we added the lithium atoms. The charge distribution in the plane was also analyzed.

With the Discovery of fullerenes in 1985, considerable interest initiated regarding the physical chemical properties of these substances, including the superconductivity of doped species [1].

Many properties of the fullerenes have been investigated experimentally and theoretically, such as electronic structure, vibrational states and chemical reactivity of the atoms and molecules. Experiments with collision energies could insert atoms in the structure of the fullerenes. The formation of composites of the type M_xC_{60} with various alkaline metals (electron donors), where M = Li, Na, K, Rb, Cs, H. Solids formed by fullerenes in combination, with other elements indicate uncommon properties that may yield new scientific and technological possibilities [2].

Using the optimized coordinates of the (100) planes of fullerites of the form $[C60]_5$, $[C70]_5$, $[C80]_5$ e $[C96]_5$. We investigated the interaction between the Li atoms and the buckballs, according to Figure 1. We added 1 to 4 atoms of Li.

It was observed that there is a reduction of the Gap (HOMO-LUMO) and the energy of system as we add Li atoms compared to the (100) planes of non-interacting fullerites. The distribution of charges of the system was also analyzed.

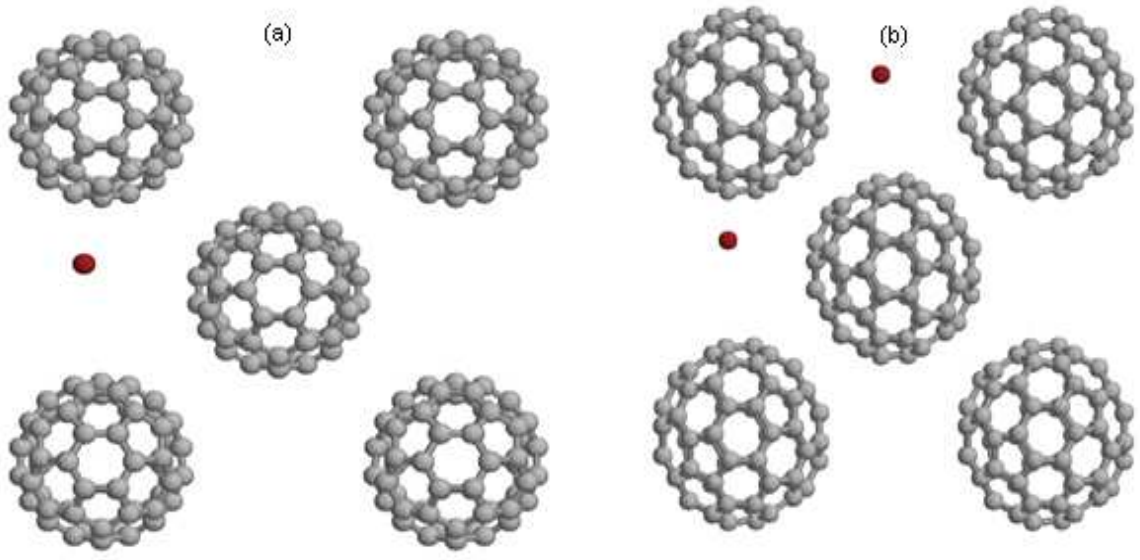

Figure 1. Model used for the interaction of the Li atoms with (100) planes of fullerites. (a) One lithium atom (b) two lithium atoms

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[2] J. D. Santos; E. Longo; M. E. Banja; V. A. A. Espinoza; J. V. Flores, C. A. Taft. J. Mol. Struct. 335 (1995).