MODELING AND INVESTIGATION OF THE HETEROFULLERENES $C_{59}X$ (X=Na, Li, Mg, Be)

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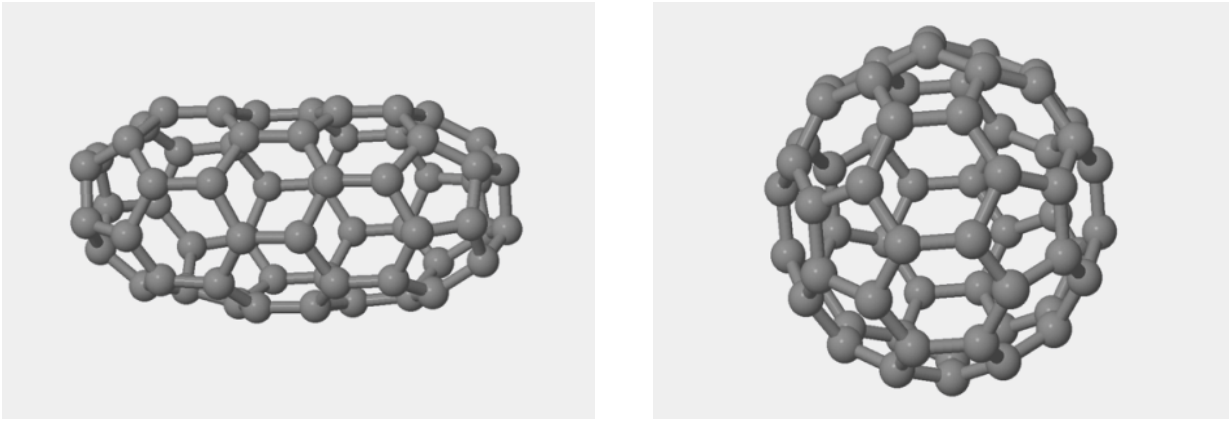
Abstract – Geometric and electronic structure of the heterofulerenes $C_{59}X$ (X=Na, Li, Mg, Be) has been studied theoretically. The main emphasis has been given to the stability of the heterefolerenes and their both HOMO and LUMO energies and ability to stabilize negative charge. Obtained results proves the application possibility of investigated heterofulerenes as components of solar cells.

In various fields of science and technology growing interest of researchers is dedicated to the variety of unusual physical and chemical properties of fullerenes and promising prospects of their possible applications.

Particularly, heterofullerenes (the type of fullerenes) attrack great attention because of their various interesting features associated with quasi-two-dimensional structure, high anisotropy and acceptor properties. So far successful heterofullerenes, containing the elements of B, N, Si, O, P, As and Ge etc., have been reported. Remarkable structural, electronic, optical, and magnetic properties were shown during the experimental and theoretical investigation of this material.

The objects of our study were structures based on C_{60} fullerene, so-called heterofullerene $C_{59}X$ (where X - the alkali metal Na, Li, Be and Mg). These system offers new possibilities for studying low-dimensional magnetic phenomena, particularly because the forces between carbon and metal elements (Na, Mg, Li, Be) appear to be very weak. In order to determine the most stable system with an implanted atom, the highest I_h and lowest C_1 symmetry of C_{60} fullerene were chosen. Heterofullerene structures of C_1 and I_h symmetries are shown on Figs. 1 and 2, respectively. The investigations were performed by B3LYP exchange – correlation hybrid functional [1] with 6-311G basis set implemented in Gausssian 03 programe package [2]. We have checked all possible different positions of implanted atoms.



(a) (b)

Figure 1 – 3D structure of C_{60} fullerene with C_1 (a) and I_h (b) symmetry

The most advantageous positions of Li, Be, Na, and Mg atoms in the system are determined, and their magnetic properties, such as the magnetizability, are investigated. By results of analysis we can say that there is a significant difference between the positions of the implanted atoms in heterofullerenes with symmetry C_1 in opposite heterofullerenes with symmetry I_h. At the same time the pure fullerenes are the most stable systems. However, results obtained indicate investigated fullerene as strong diamagnetic. On the other hand, the new modeled materials with a symmetry I_h exibited smaller HOMO-LUMO gap than that of the pure fullerenes. But this is not quite true in case of heterofullerene with symmetry C_1. Calculated values of HOMO-LUMO gap are shown in Table 1.

TABLE 1 – Values of HOMO-LUMO gap

Cage of fullerenes C_{60} with I_h symmetry		**Cage of fullerenes C_{60} with C_1 symmetry**	
Fullerene system $C_{59}X$	HOMO-LUMO gap, eV	Fullerene system $C_{59}X$	HOMO-LUMO gap, eV
where X= C (pure)	2.87	where X= C (pure)	1.31
where X= Na	1.39	where X= Na	1.33
where X= Li	1.96	where X= Li	1.28
where X= Mg	1.55	where X= Mg	1.19
where X= Be	1.63	where X= Be	1.25

It is known that HOMO-LUMO gap may be related to ability of the hetrofullerenes to generate photocurrent. Thus, smaller band gap indicate that low-energy light could be used when the above described heterofullerenes would be used to generate photocurrent.

REFERENCES

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