

CHAPTER 6

CONCLUSION

6.1 The selected the basis set

The 6-31G basis set was chosen for SCF calculations of the Li-C₆₀ system. The use of BSSE correction did not improve quality of the calculations.

6.2 Intermolecular potential function

The suitable functional forms for the exohedral and endohedral complexes are :

$$V_{\text{exo}}(x) = a \exp[-(x-b)/c]$$

and

$$V_{\text{endo}}(x) = a \exp(bx) + c$$

Good agreement between the ΔE_{FIT} and the ΔE_{SCF} was yielded only for the first function. Quality of the fit for the endohedral complex needs to be improved.

6.3 Collision energy between Li and C₆₀

By the use of maximum repulsion energies, extrapolated from the individual fit for each trajectory, it was found that the easiest pathway for firing Li to the cage of C₆₀ is to move through center of the hexagon (trajectory C6). The corresponding threshold energy is 28 eV.

6.4 Electron distribution in the Li-C₆₀ complexes

Endohedral :

When Li moves from center to surface of the cage, atomic net charge of Li decreases smoothly. Significant change of atomic net charges on carbon atoms takes place only for certain sets of carbons, which lie around the vectors parallel to the trajectories.

Exohedral :

Change of electron density on the Li in the exohedral complex is different from that of endohedral one. Donation of 2s electron from Li is nearly impossible when Li is very close to the surface. Optimal donation takes place at medium distance and decays to zero at long distance. Characteristic of the electron transfer is somehow similar to the endohedral case. Valence electron of Li doesn't transfer homogeneously to the outer surface of the C₆₀ but locates on some specific areas, covering less number of carbon atoms than the endohedral complex.

6.5 Dipole moment and stability of the Li-C₆₀ complexes

Endohedral :

When Li moves from the center to the surface of the C₆₀ cage, charge of the carbon atoms near Li increases, and potential energy and dipole moment of the complexes as well. Repulsion energies at bridging sites, B65 and B66, are higher than those of the open sites, C5 and C6. For the dipole moment, an order is altered.

Exohedral :

Interaction energy decreases as a function of C₆₀-Li distance. Dipole moment of the exohedral LiC₆₀ complexes for all trajectories increases exponentially at short distance and displays a maximum at medium distance,

then decays slowly to zero afterward. However, in term of interaction energy, trajectory C6 is still the optimal pathway for Li to approach the C_{60} .

6.6 Characteristics of the Li_nC_{60} complexes

In the Li_nC_{60} complexes, where $n = 1 - 6$ and 12 it was found that cluster size increase for higher number of Li except that for $n = 12$. The C-C and C=C bond lengths of the Li_nC_{60} complexes are significantly changed. The Li_3C_{60} complex shows the lowest HOMO-LUMO energy gap which is about 5 and 4 eV obtained from the STO-3G and the 6-31G, respectively. With the obtained energy gap for all cases, it is reliable to conclude that Li_nC_{60} system is insulator.

6.7 Suggestion for future works

Extension of the calculations for other ions

This is to examine the effect of ion sizes and charges on the changes of geometries, interaction energies, electronic structures and related properties of the complexes. It also sounds reasonable to recommend the use of the small STO-3G basis set as it has been proved that all qualities are relatively agreed with those obtained by the use of 6-31G basis set. In addition, the use of the STO-3G would also facilitate to extend the calculation to bigger alkali and alkaline earth or even transition metal ions.

Extension of the calculations using different approaches

It is interesting to extend this study using statistical Monte Carlo (MC) and Molecular Dynamics (MD) simulations on the $Li_n(C_{60})_m$ systems, where for

example $10 \leq m \leq 50$ and $10 \leq n \leq 600$. The intermolecular potential functions reported in this work can be applied. What one can learn from this investigations are location of these doped lithium atoms in the lattice and the changes of lattice parameters. These data are primarily required to understand the conductivity of the complexes. In addition, by means of MD or MC simulation, collision energy between Li and C_{60} can also be predicted. It is interesting to compare the simulation result to that obtained from the *ab initio* method.



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