

**FULLERENE BASE ACCEPTOR MATERIAL FOR ORGANIC SOLAR CELL
APPLICATION- A DFT STUDY**

Submitted in partial fulfillment of the requirements for the award of bachelor of science in chemistry

by

M.PAVITHRA (Reg.NO.40030025)

G. BHARATHI (Reg.No.40030004)



**DEPARTMENT OF CHEMISTRY
SCHOOL OF SCIENCE AND HUMANITIES**

**SATHYABAMA INSTITUTE OF SCIENCE AND TECHNOLOGY
(DEEMED TO BE UNIVERSITY)**

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JEPPIAAR NAGAR, RAJIV GANDHI

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BONAFIDE CERTIFICATE

This is to certify that this Project Report is the bonafide work of
PAVITHRA.M (Reg.no.40030025), BHARATHI.G (Reg.No.
40030004) who carried out the project entitled "FULLERENE BASE
ACCEPTOR MATERIAL FOR SOLAR CELL
APPLICATION- A DFT STUDY" under my supervision from
August 2022 to April 2023.

Amirta Paul

GUIDE

Dr. AMIRTA PAUL
ASSITANT PROFESSOR
DEPARTMENT OF CHEMISTRY

J. Karthikeyan
HEAD OF THE DEPARTMENT
DEPARTMENT OF CHEMISTRY
SATHYABAMA
INSTITUTE OF SCIENCE AND TECHNOLOGY
(DEEMED TO BE UNIVERSITY)
Sathyabama Nagar, Rajiv Gandhi Salai
Chennai - 600 119

Submitted for Viva voce Examination held on 08.05.2023

Ramiris

Internal Examiner

V. Subramanian

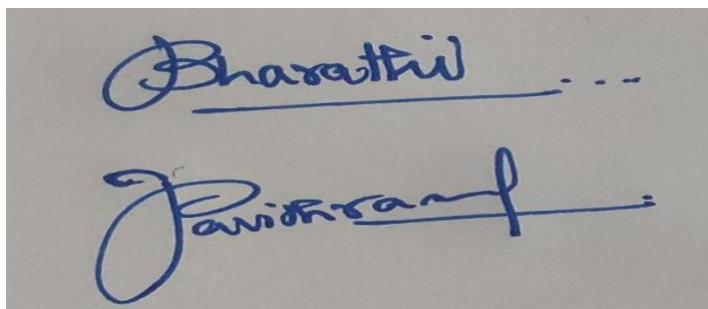
External Examiner

DECLARATION

We PAVITHRA.M (Reg.No. 40030025), BHARATHI.G (Reg.No. 40030004), hereby declare that the project Report entitled “**FULLERENE BASE ACCEPTOR MATERIAL FOR SOLAR CELL APPLICATION- A DFT STUDY**” done by us under the guidance of **Dr. AMIRTA PAUL Ph.D.**, Associate Professor, Department of Chemistry, Sathyabama Institute of science and Technology is submitted in partial fulfilment of the requirements for the award of Bachelor of Science degree in Chemistry.

DATE: 08.05.2023

PLACE: CHENNAI

A photograph of two handwritten signatures in blue ink on a light-colored background. The top signature is 'Bharathi' followed by three dots and a horizontal line. The bottom signature is 'Pavithra' followed by a horizontal line.

SIGNATURE OF THE CANDIDATES

M.PAVITHRA (40030025)

G. BHARATHI (40030004)

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M.PAVITHRA (40030025)

G. BHARATHI (40030004)

ABSTRACT

The ultrafast photo-induced electron transfer from polymer to fullerene, low cost, light weight, large- area application, semitransparency, new market opportunities (e.g., wearable PV) resulted in the flourish of OSCs. Extensive research on the Power conversion efficiency (PCE) has led to development of highly efficient bulk heterojunction (BHJ) single and multijunction organic solar cells with PCEs > 15%.

In recent years a lot of research has been done to increase the PCE of the BHJ-OSCs but majority of them focuses on the optimization of donors therefore less attention has been given to fullerene-based acceptor materials. Although fullerene derivatives have been widely used, the structural optimization still to be needed to increase the compatibility with the P3HT donors. Bearing in mind the importance of fullerene as an acceptor we have done a systematic study of fullerene modified derivatives that have high PCE and those that have low PCE. The structures of the modified fullerene derivatives that has been taken from [1] was optimized using Gaussian software and the calculations were done. This study will be of use for future researches based on fullerene derivatives as an acceptor for BHJ-OSCs.

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LIST OF ABBREVIATION

S.NO	ABBREVIATION	EXPANSION
1.	OSC	Organic solar cell
2.	TiO ₂	Titanium Oxide
3.	DFT	Density Functional Theory
4.	HOMO	Highest Occupied Molecular Orbital
5.	LUMO	Lowest Unoccupied Molecular Orbital
6.	IR	Infra Red
7.	UV-vis	Ultra Violet-visible
8.	JSC	Short Circuit Current
9.	VOC	Open Circuit Voltage
10.	BHJ	Bulk hetereojunction
11.	PCE	Power conversion efficiency

CHAPTER 1

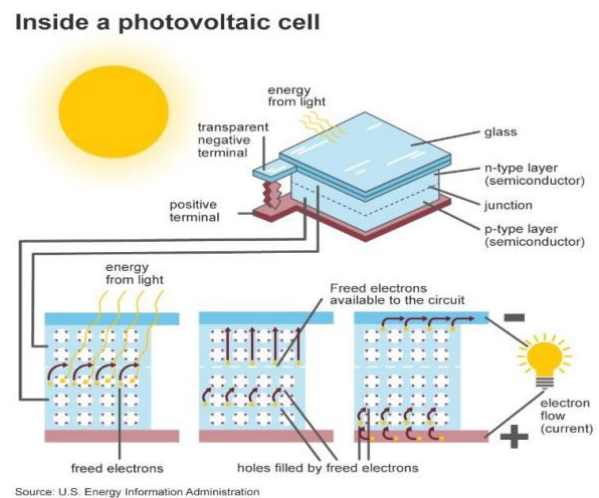
INTRODUCTION:

1.1 OVERVIEW

Solar cell is a device which converts the solar radiation into current. Electronic revolutions that happened in the last fifty years led to increase in energy demand which was satisfied by using non-renewable energy resources. This caused depletion of fossil energy resources and increased greenhouse gas emission which induced global warming and sudden natural calamities. To avoid this, we had to switch to an eco-friendlier renewable energy resource, the solar energy. To harvest this energy, we use the solar cell. Thus, solar cell will play a key role in control of environmental deteriorations.

It's said that using a WWS (wind water sun) system ~3,800,000 5 MW wind turbines, ~49,000 300 MW concentrated solar plants, ~40,000 300 MW solar PV power plants, ~1.7 billion 3 kW rooftop PV systems, ~5350 100 MW geothermal power plants, ~270 new 1300 MW hydroelectric power plants, ~720,000 0.75 MW wave devices, and ~490,000 1 MW tidal turbines can power a 2030 WWS world that uses electricity and electrolytic hydrogen for all purposes.

The solar cell is in the form of p-n junction. The light that is incident on the solar cell gets absorbed by the solar cell when it has a certain wavelength -the visible light with longer wavelength (those that have less photon energy) are more efficient with photovoltaic cells than ones that have shorter wavelength and is more energetic thus red light produces more electricity than other colors. The absorbed solar energy interacts with the constituents of the semiconducting part of the solar cell. As a result, holes and electrons are formed these are known as minority charge carriers these move to their respective electrodes. The flow of these electrons results in production of electricity



Source: U.S. Energy Information Administration

FIG 1

The polymer solar cell has gained a lot of attention in

recent days because of the following factors first its active layer is between 150 and 200 nm thick, resulting in a significantly lower use of materials compared with a traditional silicon solar cell. Second the use of cheap, abundant materials like plastics and aluminium and the possibility of processing the active material using existing cost-effective and low-energy printing or coating techniques results in a significantly lower price than silicon-based solar cells and less environmental impact. Thirdly the polymer solar cell has environmental advantages compared with other solar cells. Lastly compared with silicon-based solar cells the production is more energy efficient, and they do not have the problems with heavy metals and chemicals that other (nano) solar thin films have.

[6] The polymer solar cell is a layered structure consisting of three main layers

- i. A transparent front electrode,
- ii. An active layer (which is the actual semiconducting polymer material) and
- iii. A back electrode printed onto a plastic substrate

Polymer solar cells are classified on the basis of the active layer preparation into mono layer, bilayer, BHJ, tandem, and inverted solar cells

For every polymer solar cell except monolayer, we need a donor and an acceptor for the donor layer conjugated polymer or small molecule is most widely used and for acceptor layer polymer, small molecule, perylene diimide, and fullerene derivatives are extensively used.

The ultrafast photo-induced electron transfer from polymer to fullerene, low cost, light weight, large- area application, semitransparency, new market opportunities (e.g., wearable PV) resulted in the flourish of OSCs. Extensive research on the Power conversion efficiency (PCE) has led to development of highly efficient bulk heterojunction (BHJ) single and multijunction organic solar cells with PCEs > 15%. This has been achieved through the development of new photoactive materials, interfacial modification and device architecture design. The limited solubility of pristine C60 showed the lower performance in OSCs, hence, it is compulsory to find soluble fullerene derivative for efficient OSCs. This paves the way for the synthesis of new fullerene derivatives, such as PC61BM, which is highly soluble in aromatic solvents, and efficient electron acceptor than the pristine C60. In OSCs, P3HT polymer and PC61BM are most widely used donor and acceptor respectively.

To commercialize the low cost osc, PCE should be improved. The PCE can be improved by tailoring the donor and acceptor material with the wide and strong absorption in UV–vis to NIR region, appropriate energy levels, material miscibility, improved charge transporting properties, open circuit voltage (V_{OC}), fill factor (FF) and short circuit current density (J_{SC}). By doing these numerous functionalized fullerene derivatives have been reported with improved efficiency.

In recent past, Chen et al. reported a record high PCE of ~10% for a single junction BHJ OSCs, which was obtained for the PTB7-Th polymer with PC71BM ([6,6]-phenyl-C71-butyric acid methyl ester) acceptor. Similarly small molecule based single-junction BHJ-OSCs with PC71BM reached a record high PCE of ~10%. In the case of tandem solar with PC61BM and PC71BM as acceptor layers reached PCE of ~15%. Similarly, fullerene free bilayer and BHJ solar cell based on small molecule and PCDTBT polymer acceptors showed an improved efficiency of ~8.4% and ~10% respectively. Heliatek achieved the highest certified efficiency of ~12% in December 2013, for a multi-junction solar cell. Though, some highly conjugated n-type polymers, and small molecules performed better than the fullerene derivatives, but PC61/71BM acceptors still the cornerstone of all fullerene derivatives

In recent years a lot of research has been done to increase the PCE of the BHJ-OSCs but majority of them focuses on the optimization of donors therefore less attention has been given to fullerene-based acceptor materials. Although fullerene derivatives have been widely used, the structural optimization still to be needed to increase the compatibility with the P3HT donors. Bearing in mind the importance of fullerene as an acceptor we have done a systematic study of fullerene modified derivatives that have high PCE and those that have low PCE. The structures of the modified fullerene derivatives that has been taken from [1] was optimized using Gaussian software and the calculations were done. This study will be of use for future researches based on fullerene derivatives as an acceptor for BHJ-OSCs.

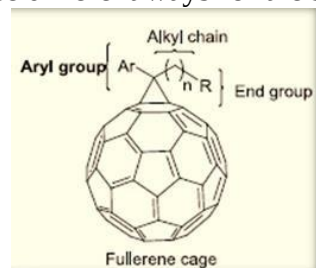
1.2. FULLERENE

Fullerene is the third stable allotrope of carbon it is also called as Buckminster fullerene is any of a series of hollow carbon molecules that form either a closed cage (“buckyballs”) or a cylinder (carbon “nanotubes”). Which was first discovered in 1985 by Sir Harold W. Kroto of the United Kingdom and by Richard E. Smalley and Robert F. Curl, Jr., of the United States. They obtained these cage-like molecules composed of 60 carbon atoms (C_{60}) joined together by single and double bonds to form a hollow sphere with 12 pentagonal and 20 hexagonal faces with 60 bonds out of these 30 conjugated double bonds by vaporising graphite using laser in an atmosphere of helium gas. Higher fullerenes like C70, C74, C76, C78, C80, C82, C84, and etc., are also present in the fullerene family.

1.2.2 FULLERENE MODIFICATIONS

We have used basic fullerene derivatives that has been modified in three different ways for the study

- i. Modifications on the aryl group
- ii. Modifications on the alkyl chain length and
- iii. Modifications on the end group



SOURCE [1] FIG 2 Fullerene based acceptors for efficient bulk heterojunction organic solar cell applications

Ramasamy Ganesamoorthy, Govindasamy Sathiyam, Pachagounder Sakthivel

1.3. CLASSIFICATION OF SOLAR CELLS

Solar cells are mainly classified into three types non-organic based solar cells, organic based solar cells and hybrid solar cell which is made by a mixture of organic and inorganic materials.

(SOURCE [1]) FIG 3 Fullerene based acceptors for efficient bulk heterojunction organic solar cell applications

Ramasamy Ganesamoorthy, Govindasamy Sathiyam, Pachagounder Sakthivel

1.3.1 Non-organic solar cells

These are made by silicon or non-silicon-based materials. Silicon based solar cells are significant due to its higher efficiency and market availability. Pure silicon single crystal or multi crystals are used in the preparation of silicon based solar cells.

1.3.1.1 Single crystal Si solar cells

The single crystal silicon solar cell plays an important role in the solar cell market due to its high PCE than other silicon solar cell. But it was very costly and high energy was needed for the production of good quality single crystals without any imperfections. This was later rectified by the amorphous or thin film inorganic solar cells, but the performance of the device was comparatively very low due to imperfection

1.3.1.2. Thin film solar cells

Even though it is lightweight and cost effective its performance is lower than the crystalline solar cells. Amorphous silicon solar cells are most often used in scientific calculators, and garden lamps. Cadmium telluride (CdTe), copper indium gallium diselenide (CIGS), amorphous thin-film silicon, and etc., are commercially available thin film solar cells.

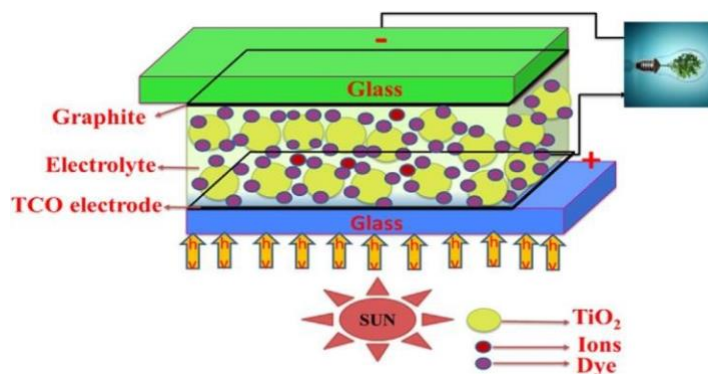
1.3.2 Organic solar cell

Emerging organic solar cells are called as third generation photovoltaic cells because, these materials are the latest entry into the solar cell field. Third generation cells are classified into several types such as,

1.3.2.1. Dye sensitized solar cell (DSSC)

The working of DSSC is as follows

- i. Light absorption and excitation of an electron.
- ii. Electron transfer (diffusion) from dye to the valence band of the metal electrode TCO/ITO
- iii. Diffusion of electron to the TiO_2
- iv. Electron moves towards the rheostat
- v. The electron reaches the conduction band of iodine
- vi. The redox step here I_3^- is converted into 3I^- or reduction of iodine at the counter electrode
- vii. Diffusion in the electrolyte and regeneration of the oxidized dye.



(Source [1] Fullerene based acceptors for efficient bulk heterojunction organic solar cell applications

Ramasamy Ganesamoorthy, Govindasamy Sathiyar, Pachagounder Sakthivel) DSSC's systematic diagram FIG 4

1.3.2.2. Polymer or plastic solar cells

They are classified into five types based on device fabrication methods,

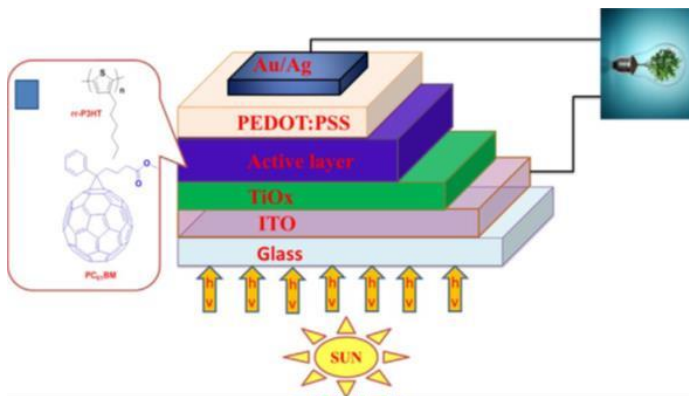
- i. Monolayer solar cells
- ii. Bilayer solar cells
- iii. BHJ solar cells
- iv. Inverted solar cells
- v. Tandem solar cells

1.3.2.2.1 Monolayer solar cell

The Monolayer solar cell is the starting point of the OSCs. Either electron donating or electron accepting material is sandwiched between high and low work function electrodes. When the light strikes on the active layer it emits an electron to the surface of the electrode. Due to lower absorption, it excites a small fraction of the electron hence it reduced the overall performance below 1%. In recent days enormous improvement has

come in the single layer solar cells, various single layer materials are used in the solar cells, which showed the PCE less than 2%. This difficulty was further rectified by bilayer solar cells.

1.3.2.2.2. Bilayer solar cell



Bilayer solar cells are prepared by coating the electron donating p-type layer and electron accepting n-type layer one after another over the PEDOT: PSS (poly-3,4-ethylenedioxythiophene: polystyrene sulfonate) modified ITO (indium tin oxide) glass electrode. In the bilayer solar cells both, donor and acceptor units are present in the active layer, which improved the absorption efficiency of the OSCs. Though improved

[Fullerene based acceptors for efficient bulk heterojunction organic solar cell applications](#)

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absorption and PCE than mono layer, the interfacial area between the donor and acceptor is very low, which limits the generation of exciton. This defect was rectified by the BHJ-OSCs device structure.

(SOURCE [1] [Fullerene based acceptors for efficient bulk heterojunction organic solar cell applications](#))

[Ramasamy Ganesamoorthy, Govindasamy Sathiyam, Pachagounder Sakthivel](#)) Bilayer OSCs schematic diagram FIG 5

1.3.2.2.3. BHJ solar cell.

In the BHJ device a blend or mixture of donor and acceptor molecules in same or different solvents were used to form a bi-continual layer. Bicontinuous three-dimensional interpenetrating network yielded an increased D-A interface, which is the necessary criteria for the effective exciton dissociation. Main difference between the traditional bilayer, and BHJ is the wide area of interfacial layer between the active layer materials.

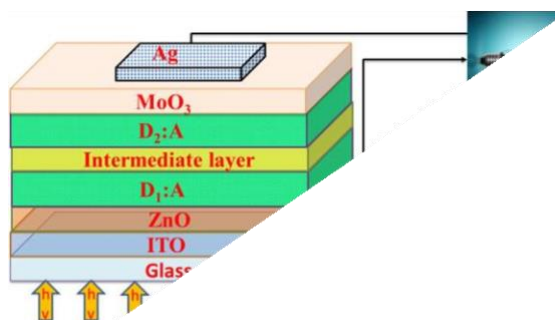
1.3.2.2.4. Inverted solar cell.

The long-time applicability of conventional solar cells is not possible due to the damage caused by the oxygen and moisture in the air to the electrodes which was rectified by the inverted device structure. In the new

inverted device structure, high work function metal or metal oxides are used as a cathode which is the top electrode and the low work function metal is used as an anode. The inverted OSCs configuration not only achieved an impressive PCE of ~10.08%, but also exhibited an exceptional device lifetime without any external coating.

1.3.2.2.5. Tandem solar cell

Multijunction or tandem solar cells are two or more solar sub cells connected in series manner. The tandem organic solar cells high theoretical PCE of ~20% which is with the conventional inorganic solar cells, of the tandem solar cell was expensive techniques.



prepared by or parallel showed very comparable main drawback manufacturing

(SOURCE [1] Fullerene based acceptors for efficient bulk heterojunction organic solar cell applications Ramasamy Ganesamoorthy, Govindasamy Sathiyar, Pachagounder Sakthivel) Tandem OSCs schematic diagram. FIG 7

Pure organic solar cell maximum PCE is ~12%, but for the commercial device, it is less than the ~3%, but in the case of inorganic solar cell it is reversible, hence several scientific groups tried in a different way to improve the efficiency of solar cell, so they combined inorganic and organic solar cells and constructed a new device called hybrid solar cells, targeting a better power conversion efficiency in these hybrid systems.

1.3.3.1. Perovskite solar cells

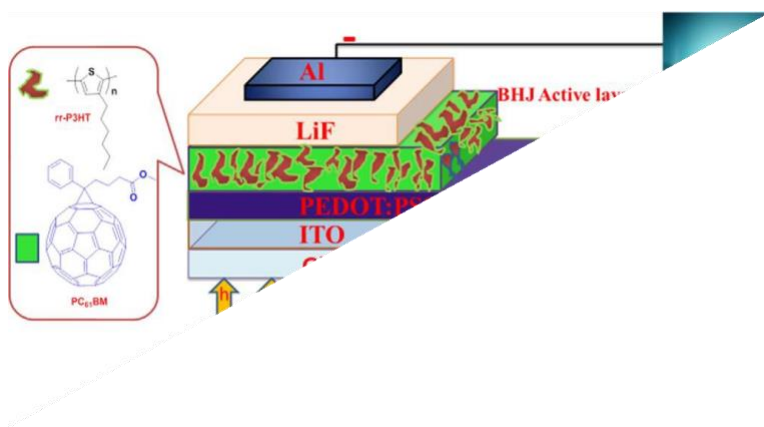
The main competitor to the inorganic solar cell was the Perovskite solar cell due to higher potential to produce comparable PCE with the conventional inorganic solar cells. Solar cell applicable Perovski mineral is a crystal made of calcium titanium oxide. General molecular formula of Perovskite solar cell material is ABX_3 , where A and B are cations coordinate with 12 and 6 'X' anions, which resulted in the formation of cuboctahedral and octahedral geometries respectively with identical crystal structure with calcium titanate.

1.4. WORKING OF BHJ-OSCs

The structure consists of a blend of P3HT donor and PC61BM was sandwiched between the PEDOT: PSS coated high work function electrode (anode) and low work function electrode (cathode).

The manner in which is a BHJ-OSC works is as follows

- i. Absorption of light by the photoactive layer
- ii. Excitation of electrons from HOMO level of either acceptor or donor to LUMO level by sunlight absorption process. This results in the creation of exciton which is electrostatically bond hole and electron pair
- iii. Diffusion of exciton to the D-A interface.
- iv. Disassociation of exciton into electron and hole
- v. The separated electron and hole will move towards their corresponding electrodes.



(SOURCE [1] Fullerene based acceptors for efficient bulk heterojunction organic solar cell applications Ramasamy Ganesamoorthy, Govindasamy Sathiyam, Pachagounder Sakthivel) BHJ-OSCs schematic diagram.

1.5 DENSITY FUNCTIONAL THEORY:

Density-functional Theory (DFT) is a computational quantum mechanical modelling method used in physics, chemistry and materials science to investigate the electronic structure (or nuclear structure) (principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases. Using this theory, the properties of a many-electron system can be determined by using functionals, i.e. functions of another function. In the case of DFT, these are functionals of the spatially dependent electron density. DFT is among the most popular and versatile methods available in condensed-matter physics, computational physics, and computational chemistry.

DFT has been very popular for calculations in solid-state physics since the 1970s. However, DFT was not considered accurate enough for calculations in quantum chemistry until the 1990s, when the approximations used in the theory were greatly refined to better model the exchange and correlation interactions. Computational costs are relatively low when compared to traditional methods, such as exchange only Hartree–Fock theory and its descendants that include electron correlation.

Density functional theory (DFT) calculations were applied to estimate the molecular geometry, electronic distribution of frontier molecular orbitals (HOMO and LUMO) and optical specification.

1.5.1 First principle of DFT:

The major advantage of this approach is transition from a wave function, depending on the coordinates of all electrons to a charge density depending on three spatial coordinates only.

1.5.2 What problems does DFT solve?

Atomistic modeling in general, and DFT calculations in particular, provide significant value to researchers and scientists working with chemicals, electronic materials, etc., in two distinct ways:

1. Since it can handle essentially any element in the periodic table in any kind of atomic arrangement, without the need for experimental input parameters, DFT has strong predictive power, even for completely new molecules or materials. In this way, atomistic simulations can reduce development time and cost by down-selection of promising material candidates prior to going into the lab and dealing with expensive and possibly hazardous chemicals with unknown properties and behavior. Using high-performance computer (HPC) clusters, a single person can screen hundreds or even thousands of materials in parallel, vastly outnumbering the number of experiments a human can perform at the same time.
2. Second, DFT calculations are used to help understand how materials and devices behave and operate under different conditions. A trained DFT user can correlate measurement data with simulation results to draw conclusions about the physical origin of certain effects observed in the material or device, but which cannot readily be explained with simple models. Such insight is crucial in order to fully exploit the effects and material in question, and even more so in order to, for instance, scale down device dimensions or optimize material choices or process conditions.

Thus, thanks to its predictive capabilities and atomistic quantum-mechanical nature, DFT is a crucial tool for technology pathfinding, to explore novel materials and exotic physical phenomena, years prior to a first test device being manufactured or even before new material has been fully characterized experimentally!

1.6 ACCURACY CONSIDERATIONS:

A DFT calculation adds an additional step to each major phase of a Hartree-Fock calculation. This step is a numerical integration of the functional (or various derivatives of the functional). Thus in addition to the sources of numerical error in Hartree-Fock calculations (integral accuracy, SCF convergence, CPHF convergence), the accuracy of DFT calculations also depends on the number of points used in the numerical integration.

CHAPTER 2

LITERATURE SURVEY

2.1 ORGANIC PHOTOVOLTAIC DEVICES

M.C. Scharber, N.S. Sariciftci have mentioned the key advantages of using organic photovoltaic devices [8]

The following key advantages of organic photovoltaic (OPV) devices have been identified:

- 1.Low weight and flexibility of the PV modules.
- 2.Semitransparency.
- 3.Easy integration into other products.
- 4.New market opportunities, e.g., wearable PV.
- 5.Significantly lower manufacturing costs compared to conventional inorganic technologies.
- 6.Manufacturing of OPV in a continuous process using state of the art printing tools.
- 7.Short energy payback times and low environmental impact during manufacturing and operations.

2.2 BHJ's

Yu et al. introduced a new device structure namely, bulk heterojunction (BHJ) structure, which is the most widely used and successful device structure in the OSCs field. In the BHJ device a blend or mixture of donor and acceptor molecules in same or different solvents were used to form a bi-continual layer. Bicontinuous three-dimensional interpenetrating network yielded an increased D-A interface, which is the necessary criteria for the effective exciton dissociation [18]

2.3 PCE

Recently, Chen et al. reported a record high PCE of ~10% for a single junction BHJ-OSCs, which was obtained for the PTB7-Th polymer with PC71BM ([6,6]-phenyl-C71-butyric acid methyl ester) acceptor.[19]

CHAPTER 3

AIM AND SCOPE

3.1 AIM:

To find out the efficiency of solar cell using fullerene base acceptor material for organic solar cell application.

3.2 SCOPE:

Our department has installed a new Gaussian software which is used for the computational chemistry studies. In this regard, our work focuses on finding the efficiency of solar cell using it on the fullerene as an acceptor. In which this solar cell can also be called as the organic Solar Cell .

3.3 OBJECTIVE OF THE STUDY:

1. Selection of fullerene structures and optimizing the corresponding structures in Gaussian software.
2. Finding HOMO–LUMO using Gaussian software
3. The final results are calculated and discussed for finding out the efficiency of solar cell.

CHAPTER 4

METHODS OF COMPUTATION

4.1 GAUSSIAN SOFTWARE:

Gaussian is a computer program used by chemists, chemical engineers, biochemists, physicists and other scientists. It utilizes fundamental laws of quantum mechanics to predict energies, molecular structures, spectroscopic data (NMR, IR, UV) and much more advanced calculations. It is released in 1970 by John Pople and his research group at Carnegie Mellon university as Gaussian70. It has been continuously updated since then and Gaussian16 is the latest version in the Gaussian series of programs. It provides state of the art capabilities for electronic structure modelling. Gaussian16 is licensed for a wide variety of computer system.

4.1.1 *What is new in Gaussian?*

Gaussian6 offers new features and performance enhancements which will enable you to model molecular systems of increasing size, with more accuracy under a broad range of real world conditions. Some of these features include.

- Model reactions of very large system with ONIOM
- Study excited state in the Gas Phase and in solution
- Additional spectra prediction
- New and enhanced methods and algorithm
- Ease of use features
- Performance improvements

4.1.2 *Advanced calculations using Gaussian6*

- ❖ Comprehensive Investigations of molecules and reactions:

Predict the structures of transition states and verify that the located stationary points are in fact minima and transition states. You can go on to compute the reaction path the following the intrinsic reaction path by following the Intrinsic Reaction Coordinate (IRC) and determine which reactants and products are connected by a given transition structure.

4.1.3 *Explore diverse chemical arenas:*

Gaussian 6 offers a variety of very accurate energy methods for predicting accurate energy methods for predicting thermochemical quantities, photochemistry and other excited states processes and solvent effects can be taken into account when optimizing structures and predicting most molecular properties.

4.2 Mulliken Population Analysis:

Mulliken atomic charges of the optimized crystal structure were carried out by B3LYP method in gas phase. The Mulliken atomic charges on carbon atoms were exhibited either positive or negative value. All hydrogen atoms were displayed a net positive charge, but H16 was gained maximum positive charge than the other hydrogen atoms, due to the presence of electronegative atom (N13). They act as acceptor atoms. Besides, all oxygen atoms of the optimized compound were shown to have negative charge, which act as donor atoms.

4.3 Frontier Molecular Orbitals:

The highest occupied molecular orbital, HOMO, and the lowest unoccupied molecular orbital, LUMO, of a molecule are called the frontier orbitals. It was Fukui who first noticed the prominent role played by HOMO and LUMO in governing chemical reactions. The positive phase is represented in red colour and the negative phase is represented in green colour.

The energy gap of HOMO–LUMO explains the charge transfer interaction within the molecule. The HOMO–LUMO analysis for fullerene structure. If there is large gap indicates that charge transfer is taking place within the molecule. The energy gap measures the kinetic stability of the molecules. A large gap implies high stability and small gap implies low stability. The high stability in turn indicate slow chemical reactivity and small gap indicates high chemical reactivity. A molecule having higher Soft value is more reactive than a molecule having smaller Soft value. In general, it can be said that the increase in softness increases chemical reactivity and increase in hardness decreases chemical reactivity. The energy gap between HOMO and LUMO has been used to prove the large efficiency of the molecule. More gaps also indicate that the molecule is less polarised and is known as hard molecule and it implies high stability being less chemical reactivity.

CHAPTER 5

RESULTS AND DISCUSSION

5.1 END ESTER GROUP MODIFICATION

The molecules were chosen from reference paper [1]. The molecules that had high PCE and low PCE were chosen, optimised, their mulliken charges and band gaps were calculated to provide a better understanding about them.

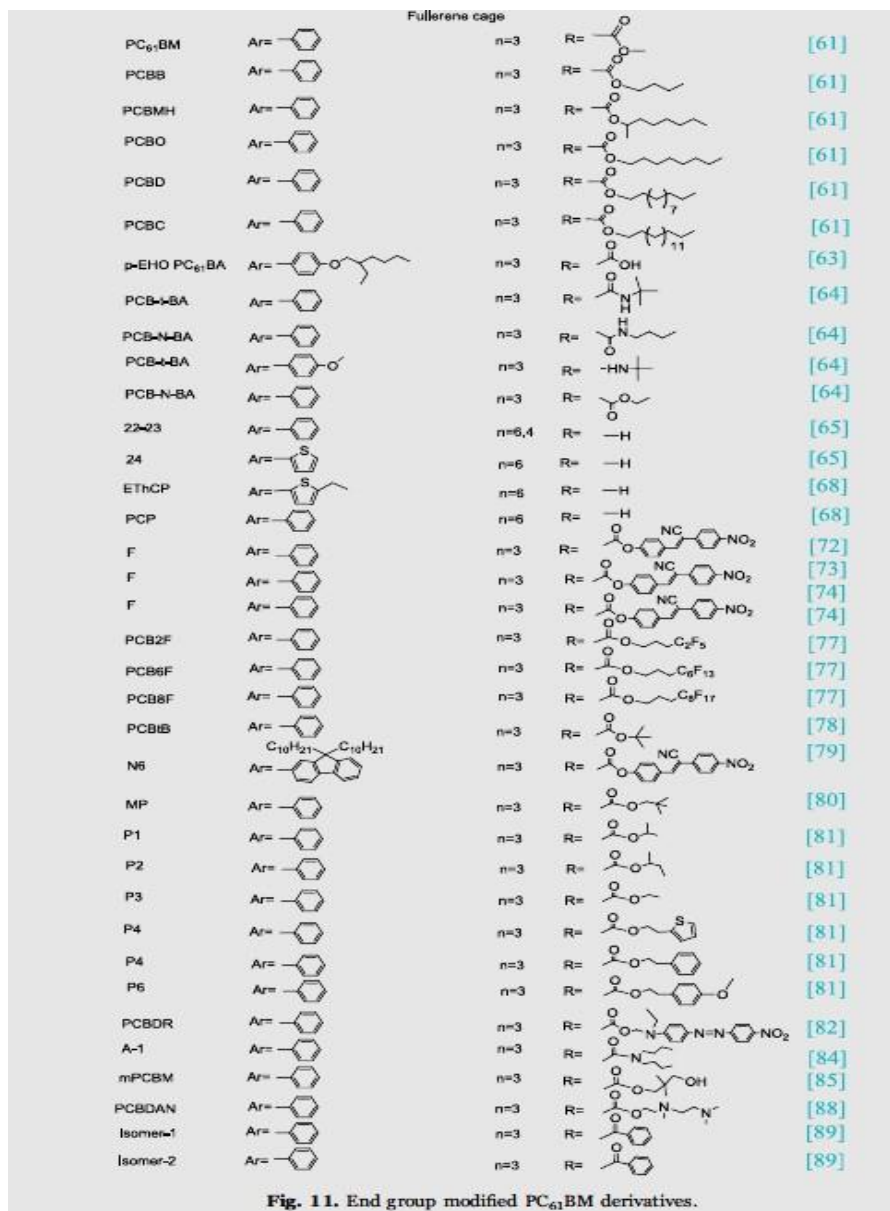


Fig. 11. End group modified PC₆₁BM derivatives.

Source [1] Fullerene based acceptors for efficient bulk heterojunction organic solar cell applications Ramasamy Ganesamoorthy, Govindasamy Sathiyar, Pachagounder Sakthivel

5.1.1 MULLIKEN CHARGES:

Since only the neutral molecules can opt for the chemical reactions, the molecules which we have taken are analyzed by Mulliken charges which gives the value zero while calculating the overall charges, this also serves as evidence that our molecules are neutral.

104	H	0.179005
105	H	0.178152
106	H	0.177811
107	H	0.161325
108	H	0.161884
109	H	0.148893
110	H	0.148439
111	H	0.146276
112	H	0.145840
113	H	0.145422
114	H	0.144939
115	H	0.143528
116	H	0.143542
117	H	0.142089
118	H	0.142400
119	H	0.142009
120	H	0.143414
121	H	0.131507
122	H	0.137192
123	H	0.142153
124	H	0.136335
125	H	0.136327
126	H	0.142233
127	H	0.130575
128	H	0.136760
129	H	0.142718
130	H	0.141299
131	H	0.140911
132	H	0.141889
133	H	0.141716
134	H	0.141372
135	H	0.141841
136	H	0.141791
137	H	0.141780
138	H	0.141729
139	H	0.141414
140	H	0.141495
141	H	0.141652
142	H	0.141590
143	H	0.140790
144	H	0.140859
145	H	0.139025
146	H	0.138982
147	H	0.135279
148	H	0.135318
149	H	0.135092
150	H	0.130917
151	H	0.130881
Sum of Mulliken charges =		-0.00000

149	H	0.141924
150	H	0.141206
151	H	0.141856
152	H	0.139222
153	H	0.138966
154	H	0.135303
155	H	0.135692
156	H	0.135505
157	H	0.131231
158	H	0.130978
159	H	0.116113
160	H	0.143492
161	H	0.140856
162	H	0.153893
163	H	0.133898
164	H	0.133711
165	H	0.138346
166	H	0.145707
167	H	0.137679
168	H	0.133781
169	H	0.141227
170	H	0.143883
171	H	0.139089
172	H	0.136211
173	H	0.134240
174	H	0.137305
175	H	0.135565
176	H	0.131112
177	H	0.131192
178	H	0.180831
179	H	0.170358
180	H	0.133574
181	H	0.173915
182	H	0.093317
183	H	0.115250
Sum of Mulliken charges =		-0.00000
Mulliken charges with hydrogens summed into		

(a) PC61BC END ESTER MODIFIED MOLECULE (b) N6 END ESTER MODIFIED FULLERENE MOLECULE

72	O	-0.201426
73	O	0.018302
74	C	0.112498
75	C	-0.315647
76	C	-0.059040
77	C	-0.505458
78	C	0.996875
79	C	-0.456993
80	C	-0.307255
81	N	-0.169089
82	C	1.079584
83	C	1.646235
84	C	-1.137498
85	C	-0.947371
86	C	-0.330275
87	C	-0.160543
88	C	0.259458
89	C	-0.725626
90	N	-0.079451
91	O	0.078695
92	O	-0.086551
93	H	0.126929
94	H	0.136738
95	H	0.128365
96	H	0.129491
97	H	0.130982
98	H	0.141176
99	H	0.153610
100	H	0.188547
101	H	0.177971
102	H	0.182619
103	H	0.182946
104	H	0.140378
105	H	0.161497
106	H	0.153338
107	H	0.128196
108	H	0.149562
109	H	0.160288
110	H	0.137557
111	H	0.148478
112	H	0.157654

Sum of Mulliken charges = -0.00000
Mulliken charges with hydrogens summed into heavy

(c) F END ESTER MODIFIED MOLECULE

61	C	1.330907
62	C	0.419286
63	C	-0.482148
64	C	-0.450744
65	C	-0.438570
66	C	-0.523862
67	C	-0.082189
68	C	-0.448274
69	C	-0.595776
70	C	-0.953915
71	C	0.218477
72	O	-0.249232
73	O	-0.065290
74	C	0.071693
75	C	-0.539110
76	H	0.126325
77	H	0.139584
78	H	0.127325
79	H	0.129052
80	H	0.129742
81	H	0.139487
82	H	0.151345
83	H	0.184964
84	H	0.177929
85	H	0.180599
86	H	0.181509
87	H	0.156780
88	H	0.155998
89	H	0.148917
90	H	0.142089
91	H	0.142647

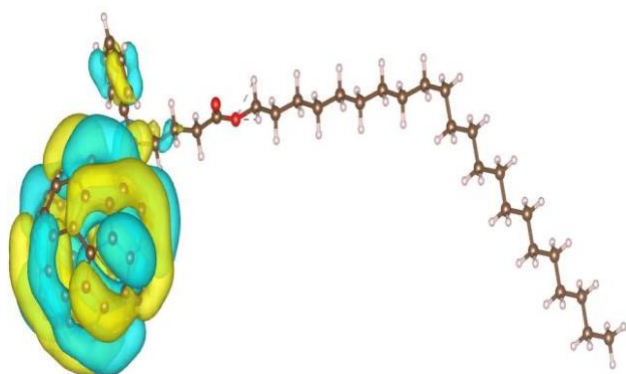
Sum of Mulliken charges = -0.00000
Mulliken charges with hydrogens summed into heavy atoms: 1

(d) P3 END ESTER MODIFIED MOLECULE

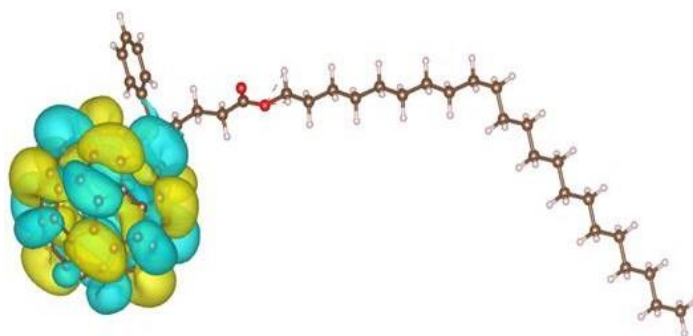
In this the molecules (b), (c), (d) have high power conversion efficiency therefore they are considered as good acceptor molecules while the molecule (a) has the least PCE among all the molecules that had their end ester group modified therefore this molecule is considered as an inefficient acceptor molecule

5.1.2 HOMO and LUMO

In order to find the energy gap, it is important to have an understanding about the HOMO and LUMO of the chosen molecules, given below are the HOMO and LUMO of the chosen molecules

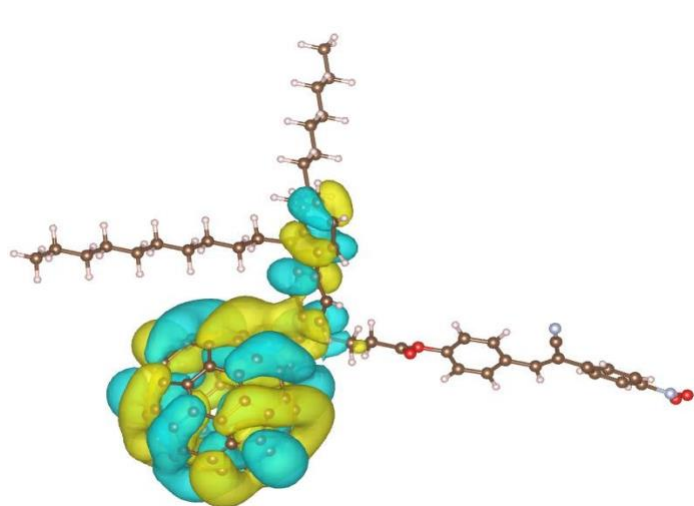


HOMO-315

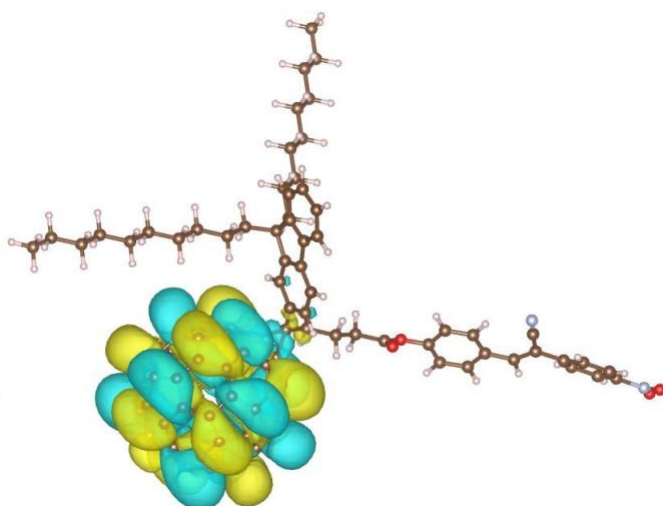


LUMO- 316

HOMO and LUMO of molecule (a)

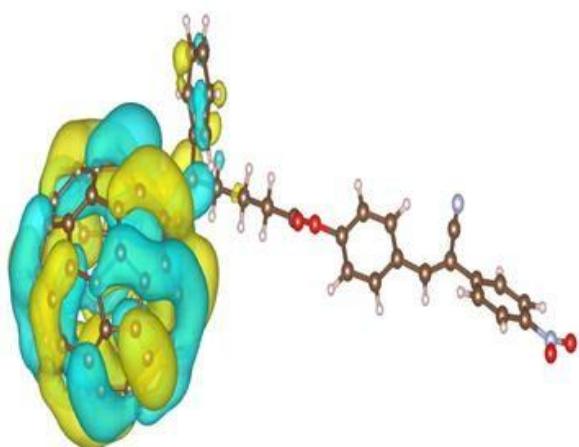


HOMO-394

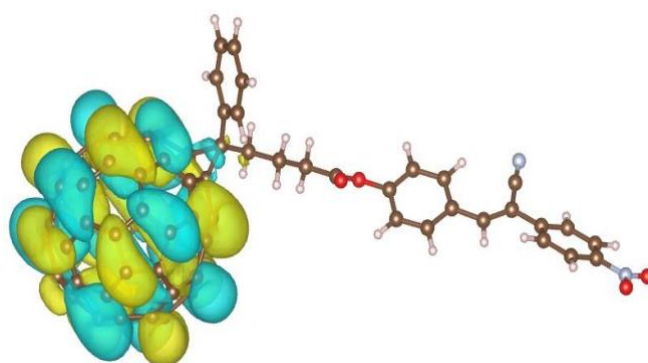


LUMO-395

HOMO and LUMO of molecule (b)

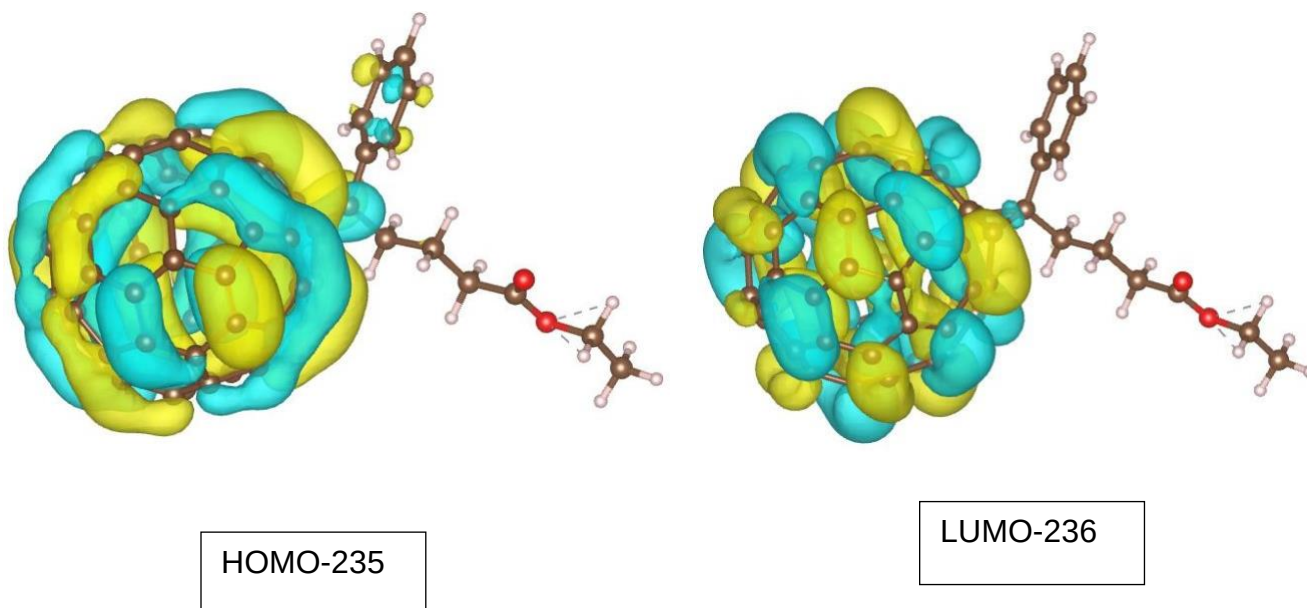


HOMO-291



LUMO-292

HOMO and LUMO of molecule (c)



HOMO and LUMO of molecule (d)

5.1.3 ENERGY GAP CALCULATION

Once the energy gap for each fullerene molecule is known, then it is easy to find the amount of energy needed for the molecule

The energy gap is calculated using the formula

$$\text{ENERGY GAP} = \text{HOMO} - \text{LUMO}$$

The highest value of HOMO and the Lowest value of LUMO are taken into consideration for calculating the energy gap

ENERGY GAP OF MOLECULE (a):

Highest value of HOMO: -0.22383

Lowest value of LUMO: -0.13091

Energy Gap: -0.35474

ENERGY GAP OF MOLECULE (b):

Highest value of HOMO: -0.23712

Lowest value of LUMO: -0.13437

Energy Gap: -0.36149

ENERGY GAP OF MOLECULE (c):

Highest value of HOMO: -0.22857

Lowest value of LUMO: -0.13546

Energy Gap: -0.36403

ENERGY GAP OF MOLECULE (d):

Highest value of HOMO: -0.22400

Lowest value of LUMO: -0.13106

Energy Gap: -0.35506

The molecule (a) is found to have the lowest energy gap.

The molecule (c) is found to have the highest energy gap.

From the above discussions it is seen that there is not much of a difference in band gap though the PCE of these molecules range from (0.11% to 4.14%)

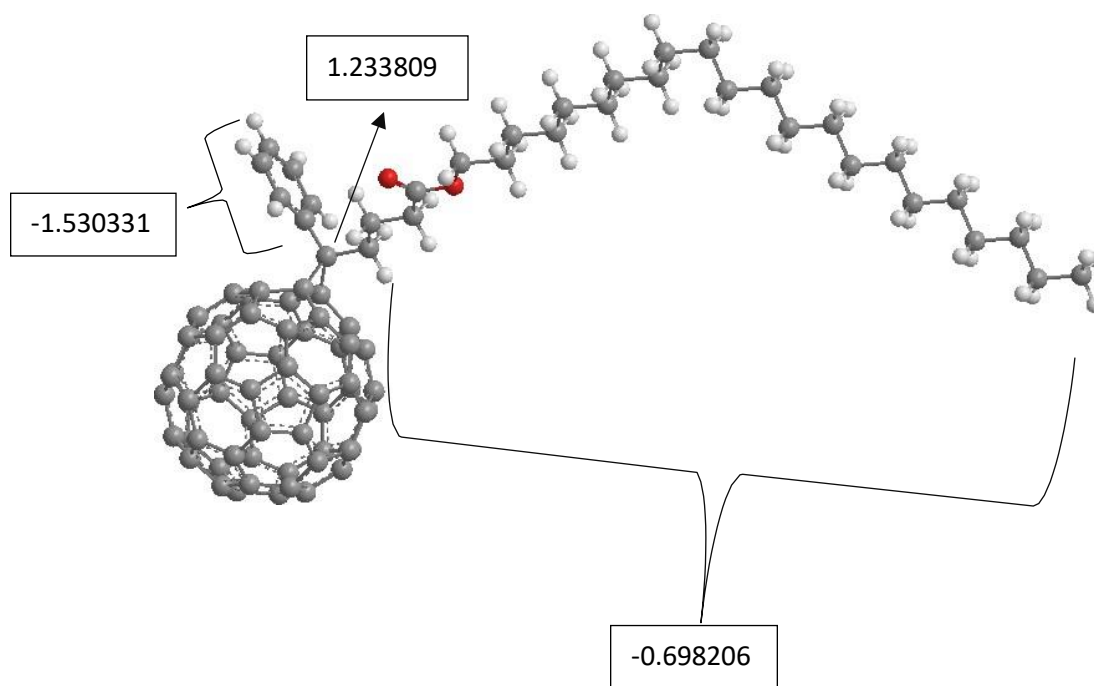
5.1.4 CHARGE CALCUALTION

There is a change in the fractional charge of the molecule due to the modifications of ligands that result in the change in electronic environment.

Therefore, the charge calculation gives a better understanding of the changes in the fractional charge when there is a modification done in the pre-existing setup.

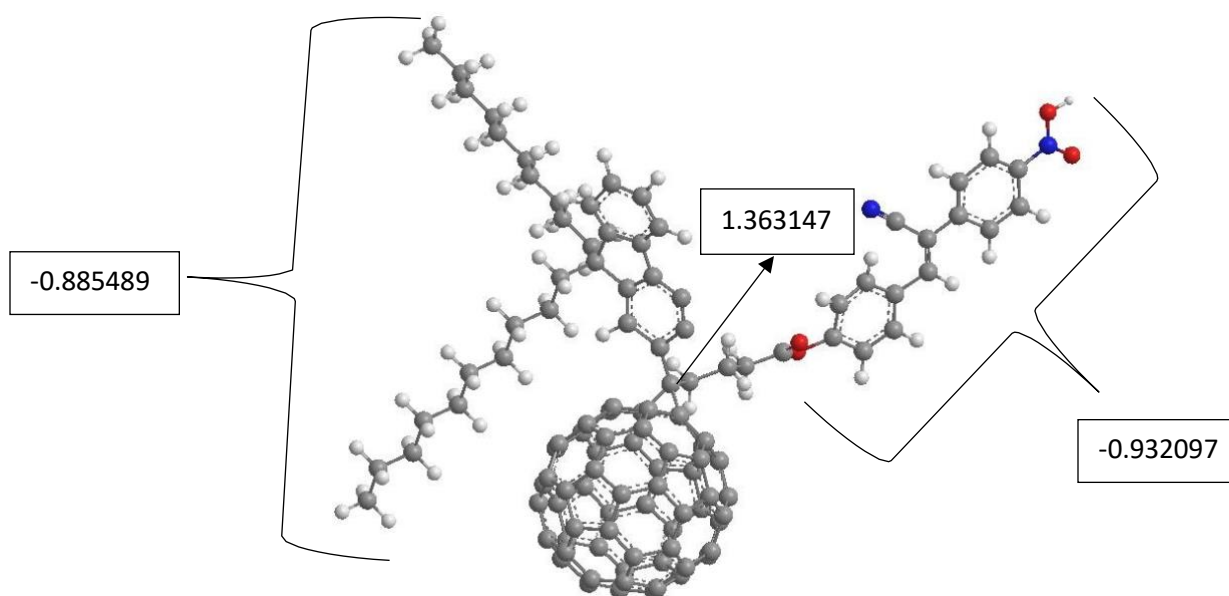
5.1.4.1 CHARGE CALCULATION OF MOLECULE (a):

The fractional value of aryl group is seen to be -1.530331, fraction charge of end ester group is -0.698206 and the fractional charge of C₆₁ is 1.233809



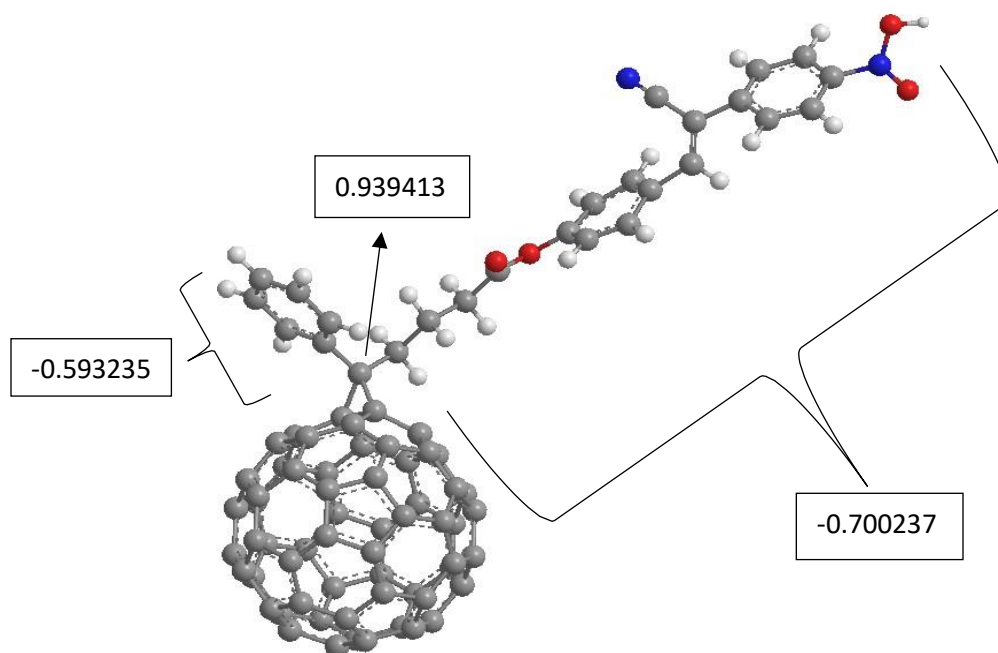
5.1.4.2 CHARGE CALCULATION OF MOLECULE (b):

The fractional value of aryl group is seen to be -0.885489, fraction charge of end ester group is -0.932097 and the fractional charge of C₆₁ is 1.363147



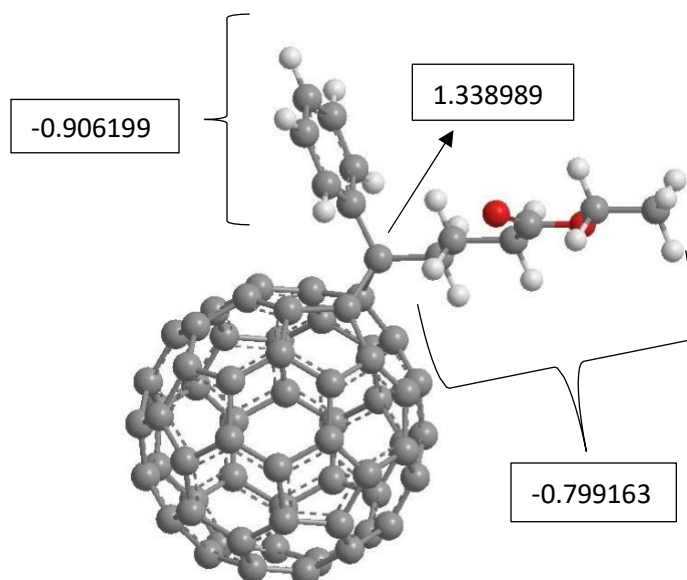
5.1.4.3 CHARGE CALCULATION OF MOLECULE (c):

The fractional value of aryl group is seen to be -0.593235, fraction charge of end ester group is -0.700237 and the fractional charge of C₆₁ is 0.939413



5.1.4.2 CHARGE CALCULATION OF MOLECULE (d):

The fractional value of aryl group is seen to be -0.906199, fraction charge of end ester group is -0.799163 and the fractional charge of C_{61} is 1.338989.



It can be seen that though the C_{61} remains attached to the same fullerene ring the modifications done in aryl group and the end ester groups brings a minute change in the charge of C_{61} .

5.2 ALKYL CHAIN LENGTH MODIFIED FULLERENE

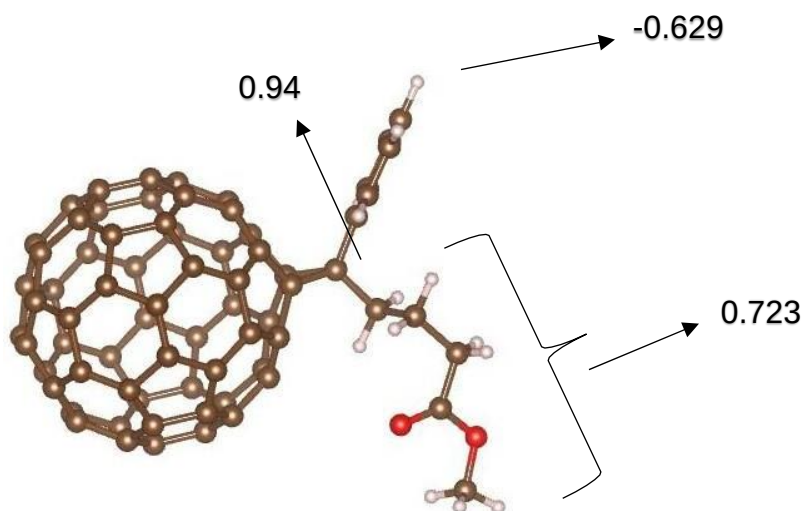
5.2.1 CHARGE CALCULATION:

The main objective of the work is achieved only by doing the charge calculation, where the fractional charges of the fullerene are considered for calculation.

The charge differences of each molecule are mentioned below.

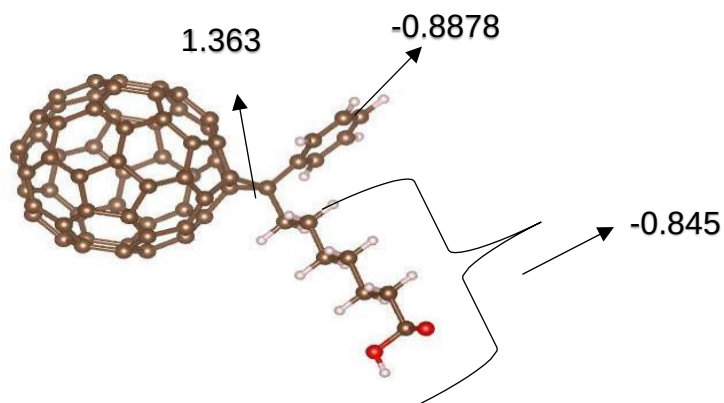
5.2.1.1 Fraction charge of structure 1:

The fraction charge will be different for different ligand. This change is due to the change in electronic environment. The fraction charge value of C61 carbon is 0.94, The fraction value of Aryl group is -0.629 and The fraction value of Chain length is 0.723. Chain group different from aryl group, that has been modified and its result increase in value.



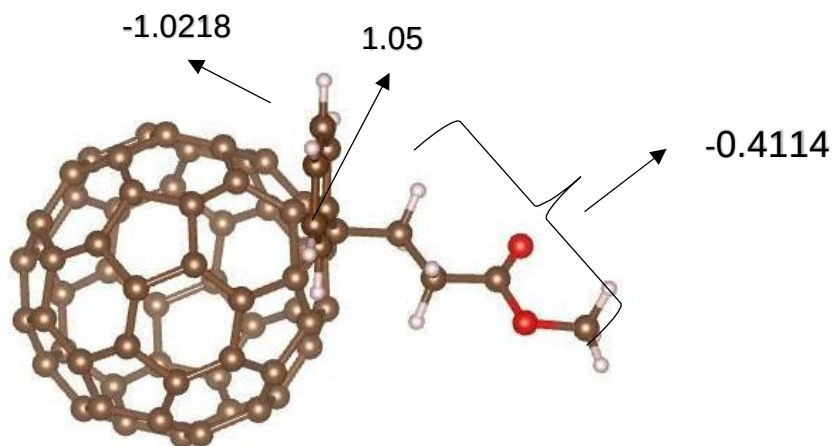
Fraction charge structure 2 :

The fraction charge will be different for different ligand. This change is due to the change in electronic environment. The fraction charge value of C₆₁ carbon is 1.363, The fraction value of Aryl group is -0.8878 and The fraction value of Chain length is -0.845. Chain group different from aryl group, that has been modified and its result increase in value.



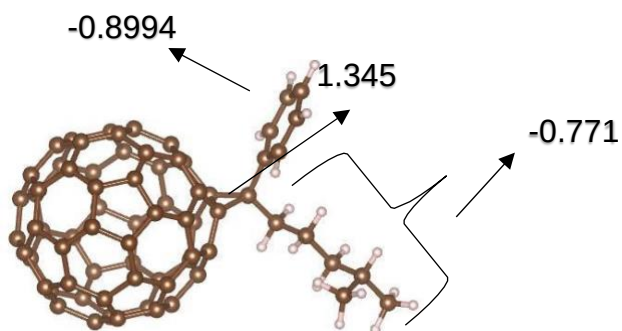
Fraction Charge structure 3:

The fraction charge will be different for different ligand. This change is due to the change in electronic environment. The fraction charge value of C₆₁ carbon is 1.05, The fraction value of Aryl group is -1.0218 and The fraction value of Chain length is -0.4114. Chain group different from aryl group. that has been modified and it's result increase in value.



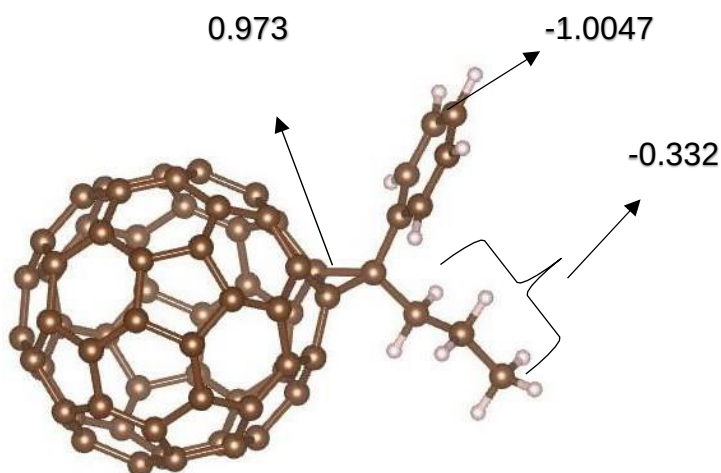
Fraction Charge structure 4:

The fraction charge will be different for different ligand. This change is due to the change in electronic environment. The fraction charge value of C61 carbon is 1.345, The fraction value of Aryl group is -0.8994 and The fraction value of Chain length is -0.771. Chain group different from aryl group, that has been modified and it's result increase in value.



Fraction Charge structure 5:

The fraction charge will be different for different ligand. This change is due to the change in electronic environment. The fraction charge value of C61 carbon is 0.973, The fraction value of Aryl group is -1.0047 and The fraction value of Chain length is -0.332. Chain group different from aryl group, that has been modified and it's result increase in value.



5.2.2 Mulliken Charges:

Since only the neutral molecules can opt for the chemical reactions, the molecules which we have taken are analyzed by Mulliken charges which gives the value zero while calculating the overall charges, this also serves as evidence that our molecules are neutral.

Mulliken charges:		
1	C	0.078657
2	C	0.020930
3	C	-0.060916
4	C	0.068340
5	C	-0.179969
6	C	0.022395
7	C	-0.274471
8	C	0.147855
9	C	-0.031531
10	C	-0.040601
11	C	-0.156918
12	C	0.222474
13	C	0.147726
14	C	-0.203152
15	C	-0.033652
16	C	0.034524
17	C	0.028236
18	C	-0.161017
19	C	0.105240
20	C	0.372191
21	C	-0.418962
22	C	0.194796
23	C	0.028321
24	C	0.193169
25	C	-0.001231
26	C	-0.185469
27	C	0.152588
28	C	-0.027325
29	C	0.245443
30	C	-0.261849
31	C	0.164891
32	C	0.143086
33	C	-0.134910
34	C	-0.357411
35	C	0.275345
36	C	-0.026247
37	C	0.073423
38	C	0.113139
39	C	-0.174231
40	C	0.085566
41	C	0.107117
42	C	0.221599
43	C	0.264969
42	C	0.221599
43	C	0.264969
44	C	-0.415337
45	C	-0.017197
46	C	-0.143284
47	C	0.134370
48	C	0.120291
49	C	0.148879
50	C	-0.294292
51	C	-0.049990
52	C	0.613032
53	C	0.263771
54	C	-0.392245
55	C	0.021499
56	C	-0.041226
57	C	-0.181320
58	C	0.030044
59	C	0.014682
60	C	-0.206847
61	C	0.940346
62	C	0.495222
63	C	-0.615709
64	C	-0.495154
65	C	-0.336542
66	C	-0.521655
67	C	-0.157021
68	C	-0.313981
69	C	-0.223996
70	C	-0.776262
71	C	-0.010164
72	O	-0.257663
73	O	-0.074276
74	C	-0.169213
75	H	0.126640
76	H	0.137994
77	H	0.126782
78	H	0.126433
79	H	0.128710
80	H	0.138483
81	H	0.147485
82	H	0.170224
83	H	0.172112
84	H	0.188292
85	H	0.189583
86	H	0.160562
87	H	0.152829
88	H	0.162951
Sum of Mulliken charges = -0.00000		

(a)

Mulliken charges:		
1	C	0.174208
2	C	0.102881
3	C	-0.117530
4	C	0.020139
5	C	-0.175765
6	C	0.052220
7	C	-0.017781
8	C	0.144801
9	C	-0.093115
10	C	-0.054217
11	C	-0.128494
12	C	0.146617
13	C	0.109687
14	C	-0.164613
15	C	0.006341
16	C	-0.071922
17	C	0.089780
18	C	-0.247662
19	C	0.047657
20	C	0.182268
21	C	-0.223694
22	C	0.281102
23	C	-0.007096
24	C	0.155090
25	C	0.059920
26	C	-0.094558
27	C	0.088360
28	C	0.001158
29	C	0.281786
30	C	-0.241525
31	C	0.138216
32	C	0.141088
33	C	-0.050038
34	C	-0.280005
35	C	0.285907
36	C	0.053224
37	C	0.029648
38	C	0.086303
39	C	-0.091634
40	C	0.053719
41	C	0.142358
42	C	0.106521
43	C	0.150288
44	C	-0.131061
45	C	-0.124705
47	C	0.120342
48	C	0.059051
49	C	0.160345
50	C	-0.214127
51	C	-0.007055
52	C	-0.168201
53	C	0.340585
54	C	-0.262545
55	C	0.057694
56	C	0.015289
57	C	-0.104873
58	C	0.003583
59	C	0.001131
60	C	-0.303751
61	C	1.363078
62	C	0.417752
63	C	-0.494166
64	C	-0.418743
65	C	-0.433229
66	C	-0.510332
67	C	-0.087849
68	C	-0.404248
69	C	-0.583437
70	C	-0.413410
71	C	-0.139580
72	C	-0.276532
73	H	0.125439
74	H	0.131943
75	H	0.127367
76	H	0.126807
77	H	0.129238
78	H	0.140893
79	H	0.151496
80	H	0.166023
81	H	0.149649
82	H	0.149400
83	H	0.147630
84	H	0.144604
85	H	0.170718
86	H	0.162594
87	H	0.148673
88	C	-0.415213
89	H	0.181924
90	H	0.182732
91	C	-0.319025
92	O	-0.270669
93	O	-0.178501
94	H	0.262491
Sum of Mulliken charges = -0.00000		
Mulliken charges with hydrogen sum		

(b)

Mulliken charges:		41 C	0.114773
1		42 C	0.133444
1 C	0.140779	43 C	0.151164
2 C	0.069191	44 C	-0.067519
3 C	-0.085379	45 C	-0.021566
4 C	0.036703	46 C	-0.126121
5 C	-0.173220	47 C	0.083700
6 C	0.076443	48 C	0.108989
7 C	-0.099875	49 C	0.137278
8 C	0.195577	50 C	-0.220546
9 C	-0.080445	51 C	0.092875
10 C	0.001700	52 C	-0.047974
11 C	-0.119360	53 C	0.301288
12 C	0.172492	54 C	-0.296468
13 C	0.097612	55 C	0.031007
14 C	-0.145804	56 C	-0.022358
15 C	-0.003925	57 C	-0.126622
16 C	-0.010321	58 C	0.038629
17 C	0.063089	59 C	-0.049384
18 C	-0.248435	60 C	-0.174091
19 C	-0.018663	61 C	1.056059
20 C	0.165726	62 C	0.526528
21 C	-0.290070	63 C	-0.644892
22 C	0.239570	64 C	-0.681128
23 C	0.023869	65 C	-0.300741
24 C	0.147877	66 C	-0.398253
25 C	-0.019064	67 C	-0.176625
26 C	-0.159571	68 C	-0.483630
27 C	0.150136	69 C	-0.499032
28 C	-0.015745	70 C	-0.100434
29 C	0.232501	71 O	-0.241005
30 C	-0.220615	72 O	-0.122059
31 C	0.144006	73 C	-0.166340
32 C	0.122656	74 H	0.128960
33 C	-0.043030	75 H	0.138319
34 C	-0.344536	76 H	0.128340
35 C	0.315521	77 H	0.127760
36 C	-0.017294	78 H	0.129709
37 C	0.011657	79 H	0.168985
38 C	0.082028	80 H	0.176295
39 C	-0.133641	81 H	0.195039
40 C	0.075076	82 H	0.190396
41 C	0.114773	83 H	0.159305
42 C	0.133444	84 H	0.160114
43 C	0.151164	85 H	0.152617
44 C	-0.067519		
45 C	-0.021566		

Sum of Mulliken charges = -0.00000

(c)

Mulliken charges:		46 C	-0.107803
1		47 C	0.085498
1 C	0.151087	48 C	0.097707
2 C	0.080152	49 C	0.164231
3 C	-0.096088	50 C	-0.189963
4 C	0.032532	51 C	0.019137
5 C	-0.176393	52 C	-0.154606
6 C	0.046144	53 C	0.287989
7 C	-0.046167	54 C	-0.278205
8 C	0.134276	55 C	0.025486
9 C	-0.063707	56 C	0.005432
10 C	-0.027193	57 C	-0.123930
11 C	-0.120159	58 C	0.012185
12 C	0.165147	59 C	0.093669
13 C	0.101321	60 C	-0.294814
14 C	-0.147812	61 C	1.345808
15 C	0.013733	62 C	0.465218
16 C	-0.041908	63 C	-0.534566
17 C	0.079247	64 C	-0.545652
18 C	-0.258548	65 C	-0.380420
19 C	0.011730	66 C	-0.409266
20 C	0.172139	67 C	-0.132029
21 C	-0.207937	68 C	-0.252996
22 C	0.237274	69 C	-0.590832
23 C	0.008884	70 C	-0.830063
24 C	0.148797	71 C	0.274114
25 C	0.022356	72 C	-0.621640
26 C	-0.135360	73 C	-0.560587
27 C	0.130696	74 H	0.125927
28 C	0.000752	75 H	0.130686
29 C	0.259163	76 H	0.126698
30 C	-0.237113	77 H	0.126065
31 C	0.120653	78 H	0.128650
32 C	0.131091	79 H	0.140950
33 C	-0.113483	80 H	0.149869
34 C	-0.285187	81 H	0.163830
35 C	0.287055	82 H	0.138993
36 C	0.016784	83 H	0.139201
37 C	0.037320	84 H	0.149959
38 C	0.077640	85 H	0.136581
39 C	-0.129412	86 H	0.138209
40 C	0.059011	87 H	0.134259
41 C	0.146245	88 H	0.137888
42 C	0.121311	89 H	0.135853
43 C	0.055555	90 H	0.140907
44 C	0.004316	91 H	0.127610

Sum of Mulliken charges = -0.00000

(d)

Mulliken charges:					
		1			
1	C	0.123791	45	C	-0.004753
2	C	0.074802	46	C	-0.106593
3	C	-0.092577	47	C	0.124753
4	C	0.033196	48	C	0.107052
5	C	-0.171999	49	C	0.151785
6	C	0.109810	50	C	-0.220365
7	C	-0.174203	51	C	0.139997
8	C	0.144510	52	C	-0.040231
9	C	-0.064602	53	C	0.266858
10	C	-0.013436	54	C	-0.354974
11	C	-0.159685	55	C	0.039532
12	C	0.195442	56	C	0.002767
13	C	0.137580	57	C	-0.111881
14	C	-0.211384	58	C	0.040017
15	C	-0.057675	59	C	-0.067422
16	C	0.024256	60	C	-0.173693
17	C	0.059729	61	C	0.973507
18	C	-0.193183	62	C	0.474386
19	C	0.074142	63	C	-0.609234
20	C	0.235470	64	C	-0.633903
21	C	-0.315641	65	C	-0.307222
22	C	0.167717	66	C	-0.413023
23	C	0.013769	67	C	-0.161242
24	C	0.151624	68	C	-0.475307
25	C	0.031094	69	C	-0.235271
26	C	-0.192799	70	C	-0.637678
27	C	0.136724	71	H	0.126146
28	C	-0.013146	72	H	0.137345
29	C	0.200680	73	H	0.126835
30	C	-0.223855	74	H	0.126579
31	C	0.175360	75	H	0.128461
32	C	0.179721	76	H	0.140213
33	C	-0.050600	77	H	0.150102
34	C	-0.344646	78	H	0.161641
35	C	0.305088	79	H	0.148377
36	C	-0.021453	80	H	0.135896
37	C	0.089051	81	H	0.138599
38	C	0.078483	82	H	0.143331
39	C	-0.171758	Sum of Mulliken charges = -0.00000		
40	C	0.071679			
41	C	0.118510			
42	C	0.145925			
43	C	0.122215			
44	C	-0.159112			
45	C	-0.004753			
46	C	-0.106593			

(e)

(e)

a)- Fig.5.2.1- Mulliken charges of structure 1

(b)- Fig.5.2.2- Mulliken charges of structure 2

(c)- Fig.5.2.3- Mulliken charges of structure 3

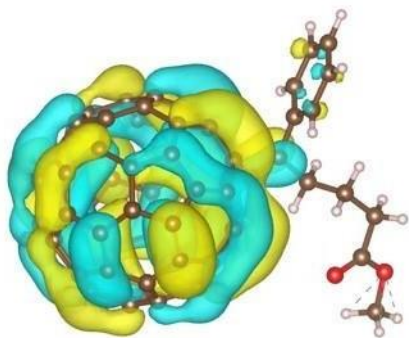
(d)- Fig.5.2.4- Mulliken charges of structure 4

(e)-Fig.5.2.5- Mulliken charges of structure 5

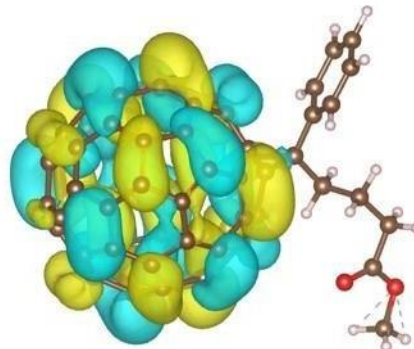
5.2.3 ANALYSING HOMO AND LUMO

To find the energy gap between the conduction band and valence band it is mandatory to find the HOMO and LUMO orbital present in each molecule.

STRUCTURE 1

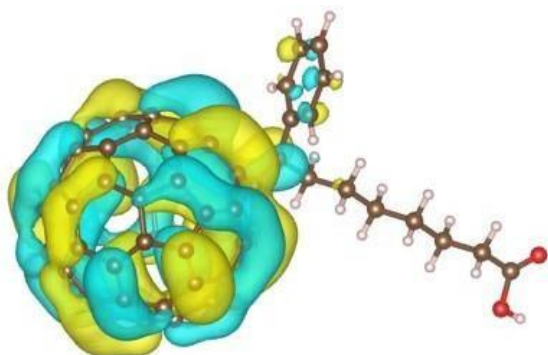


HOMO= 231

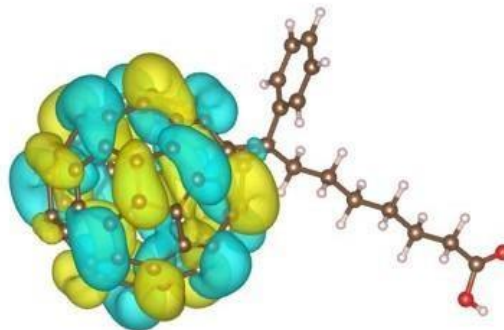


LUMO=232

STRUCTURE 2

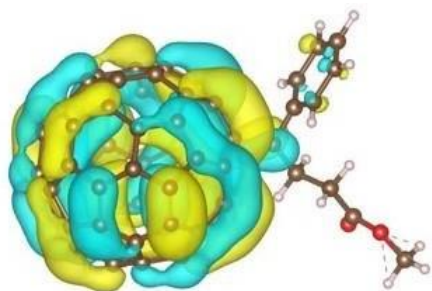


HOMO=239

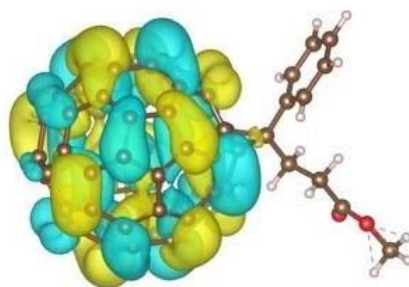


LUMO=240

STRUCTURE 3

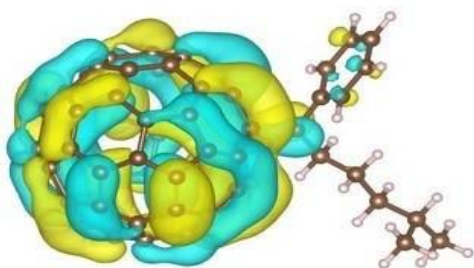


HOMO=227

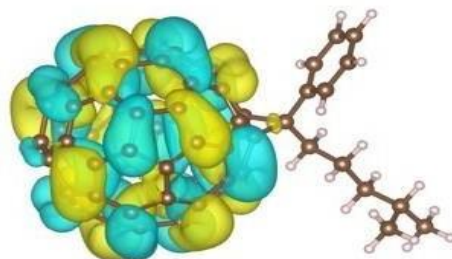


LUMO=228

STRUCTURE 4

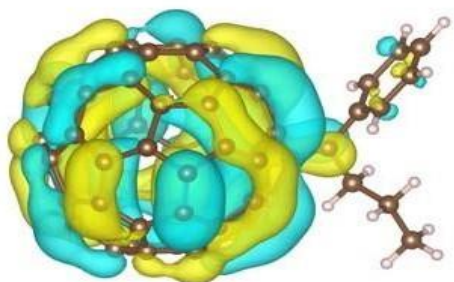


HOMO=228

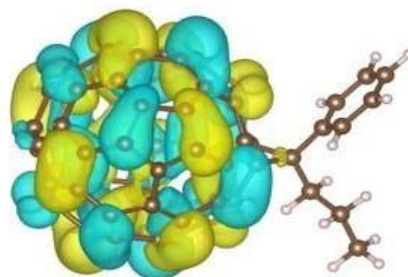


LUMO=229

STRUCTURE 5



HOMO=216



LUMO=217

5..2.4 ENERGY GAP:

Since we come to know the number of orbitals (HOMO, LUMO) present in the molecules, now it is the mandatory step to find out the energy gap. Once the energy gap for each azo molecule is known, then it is easy to find the amount of energy needed for the molecule. If the energy gap is more than the energy needed for the molecule also increases. Similarly, if the energy gap is less between two orbitals the energy needed for the molecules will also decrease.

The energy gap of the molecule is found by using the formula,

$$\text{ENERGY GAP} = \text{HOMO} - \text{LUMO}$$

The highest value of HOMO and the Lowest value of LUMO are taken into consideration for calculating the energy gap. For example, in a Structure 1 molecule, the highest value of HOMO is said to be -0.22110, and the lowest value of LUMO is said to be -0.12826 the difference between these two values gives the resultant energy gap as -0.09284. Likewise, the energy gap of the rest four molecules is found to be

Structure 2 molecule, the highest value of HOMO is said to be -0.22531, and the lowest value of LUMO is said to be -0.13236 the difference between these two values gives the resultant energy gap as -0.09295.

Structure 3 molecule, the highest value of HOMO is said to be -0.22494, and the lowest value of LUMO is said to be -0.13186 the difference between these two values gives the resultant energy gap as -0.09308.

Structure 4 molecule, the highest value of HOMO is said to be -0.22382, and the lowest value of LUMO is said to be -0.13094 the difference between these two values gives the resultant energy gap as -0.09288.

Structure 5 molecule, the highest value of HOMO is said to be -0.22397, and the lowest value of LUMO is said to be -0.13107 the difference between these two values gives the resultant energy gap as -0.0929.

CHAPTER 6

SUMMARY AND CONCLUSION

Organic solar cell (OSC) use an fullerene as an acceptor materials. Based on the ligand nature the nature of fullerene will change. This study shows the change in electron distribution due to the presence of different ligand attached to the C61 carbon with fullerene. Thus, discussed above, the following calculations can be done;

- Molecules containing fullerene were selected and optimized using Gaussian software.
- Optimized structures are analyzed using charge calculation

Based on the above data, it may be concluded that the nature of the fullerene will influence the fractional charge as well as the nature of Aryl group and End group.

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