MINOR RESEARCH PROJECT

Project Title

"STRUCTURAL, ELECTRICAL AND TRANSPORT PROPERTIES OF LONG CONJUGATED CHAIN ORGANIC MOLECULES"

No.F. MRP-6824/16 (SERO/UGC)
Link No. 6824, Comcode: TNPE004

Summary of the Report

Submitted To

UNIVERSITY GRANTS COMMISSION
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HYDERABAD-500001

Submitted By

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MINOR RESEARCH PROJECT

Titleof theProject: "Structural, Electrical and Transport properties of Long conjugated chain organic molecules"

File No.	: MRP-6824/16(SERO/UGC)
Link No.	: 6824, Dated June 2017
Comcode	: TNPE004, Department: Physics
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Project Report	: Final

Period of Report from August 2017 to July 2019

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RESEARCH PUBLICATION OF PAPERS IN A REPUTED JOURNAL IN THE FORM OF ARTICLES/BOOKS/ PRESENTATION IN SEMINARS

The work carried out by this UGC Minor Research Project is **published in two UGC approved International Journals.**

1. One paper is published in UGC approved journal, "International Journal of Scientific Research and Reviews" (IJSRR 2018, 7(4), 485-512.)
2. One paper is published in the International Journal " Journal of Computational and Theoretical Nano science" Vol. 15, 1516–1527, 2018.

Title of the paper:

Charge Density and Electrical Characteristics of1,2-di([1,1_-biphenyl]-4-yl)ethyne (DBPE) MolecularNanowire by Quantum Chemical Study

The work carried out by this UGC Minor Research Project is presented in **two National Conferences.**

1. Presented a paper in the TNSCST sponsored National conference on "Recent Advances in Physics" (NCRAP-2017) organized by NKR Govt. Arts College for women, Namakkal-637 001, Tamil Nadu on 20thseptember 2017.
2. Presented a paper in the TNSCST sponsored National Conference on "Recent Trends in Advanced Materials" organized by PGP college of Arts and science, Namakkal – 637 207,Tamil Nadu on 23rdJanuary, 2019.

OBJECTIVES OF THE PROJECT

The design of new conducting as well as insulating organic molecules will be very useful in the molecular Electronic devices. A series of conjugated organic molecules are to be selected and their Structural, Electrical and Transport properties to be studied by using Density functional Theory. The geometrical parameters, electrostatic properties obtained from computational study can be compared with synthesized compounds analyzed by various physico-chemical techniques such as UV and NMR. The molecular orbitals of the series of molecules to be analysed by density of states spectrum, and their electrical characteristics can be studied. The electrical characteristics to be analysed for the molecules with the density of states spectrum can be compared with the same obtained from the synthesised compounds by physico-chemical techniques such as spectral studies. The same methodology to be followed for thiophene and insulating molecules with poor electrical conductivity and the theoretical values can be compared with experimental results.

1. MOLECULAR ELECTRONICS

1.1 An introduction to Molecular Electronics

Molecular electronics refers to the subdivision of nanotechnology and that is responsible for development of electronic designing nano building blocks. All modern fabrication of integrated circuits and electronic devices is possible due to advancements in molecular electronics. Molecular electronics is also known as molecular-scale electronics, or moletronics. One definition is "information processing using photo-, electro, iono, magneto, thermo, mechanico or chemio-active effects at the scale of structurally and functionally organized molecular architectures. Making molecular-scale devices requires manipulating and arranging organic molecules on metal electrodes and semiconducting substrates.

The theory of molecular electronics was presented by Mark Reed. It quickly became popular among electronic device and microchip manufacturers due to its small size, light weight and flexible use. Molecular electronics includes all characteristics of conductors, insulators and semi-conductors, and also deals with the smallest scale characteristics .It deals with laws of electronics. It can control the molecular-scale properties of individual atoms of matter.

1.2 Molecular Wires

Molecular wires also known as molecular nanowires are molecular chains that conduct electric current. They are the proposed building blocks for molecular electronic devices. Their typical diameters are less than three nanometers, while their lengths may be macroscopic, extending to centimeters or more. To connect molecules, MWs need to self-assemble following well-defined routes and form reliable electrical contacts between them. Ideally, they would connect to diverse materials, such as gold metal surfaces (for connections to outside), biomolecules (for nano sensors, nanoelectrodes, molecular switches) and most importantly, they must allow branching. The connectors should also be available of pre-determined diameter and length. They should also have covalent bonding to ensure reproducible transport and contact properties .

2. QUANTUM CHEMICAL CALCULATIONS: AN INTRODUCTION

2.1 Introduction to Computational Chemistry

Quantum chemical methods have already confirmed to be valuable in discovery the molecular structure as well as reactivity. Therefore, it has become a common practice to perform quantum chemical calculations in corrosion inhibition researches. The concept of measuring the performance of a corrosion inhibitor with the assistance of computational chemistry is to look for compounds with desired properties using chemical insight and knowledge into a mathematically quantified and computerized form.

Computational chemistry has always been a significant factor in advancing the field of moletronics. Computational chemistry may be defined as the application of mathematical and theoretical principles to the solution of the chemical problems. Molecular modelling, a subset of computational chemistry, concentrates on predicting the behaviour of individual molecules within a chemical system.

The most accurate molecular models use *ab initio* or first principles electronic structure methods which are based on the principles of quantum mechanics and are generally very computer-intensive. The types of predictions possible for molecules and reactions include the following.

- Electronic transitions (UV/Visible spectra)
- Reaction pathways, kinetics and mechanisms
- Charge distribution in molecules
- Electron affinities and ionization potentials
- Vibrational frequencies (IR and Raman spectra)
- Magnetic shielding effects (NMR spectra)
- Bond and reaction energies

2.2 Quantum chemical calculations

The major goals of computational quantum chemistry are to create efficient mathematical approximations and computer programs that calculate the properties of molecules and to apply these programs to concrete chemical objects. It is usually used when a mathematical method is sufficiently well developed that it can be automated for implementation on computer. This technique often attempts to solve the non-relativistic Schrodinger equation with relativistic corrections added although some progress has been made in solving the fully relativistic Schrodinger equation. A number of approximate methods are used to achieve best trade-off between accuracy and computational costs. Present computational chemistry can accurately calculate the properties of molecules that contains up to about 40 electrons, where as for large molecules that contains a few dozen electrons is computationally tractable by appropriate methods such as DFT.

The following computer software are commonly used for computational chemistry:

- Gaussian09
- Gview
- AIMALL
- Chemdraw
- Origin
- GaussSum

In the present computational work, Gaussian09 software has been used for the entire optimization process. Further, Gview software has been used to calculate the electrostatic and transport properties in the present computational work. The GaussSum programme package has been used to plot density of states (DOS) spectrum.

3. SELECTION OF MOLECULES

To study the electrostatic and transport properties of the molecules, the molecules were optimized and studied by computational analysis with G09 by using Density Functional Theory . Then the same molecules were synthesized and their properties were studied by various experimental techniques.

The following series of conjugated organic mole were selected for first part of project work.
1.benzene 2. 1,2 diphenyl ethane 3. 1,4 Bis (Phenyl Ethyne)Benzene

4. 1,4 diphenyl Benzene 5.dipyrazino pyrazine 5. 4-bis(phenylbuta-1,3-diyn-1-yl)benzene

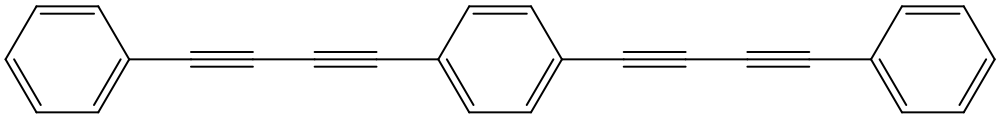
During the first part of the work, some molecules of the above were optmised and studied theoretically. Some of the above molecules were synthesized and their properties were studied by various experimental techniques.

The following series of conjugated organic mole were selected for second part of project work.
1. Cyclohexane 2.dicyclopentyl-cyclohexane 3.Thiophene 4. 2,2' bithiophene

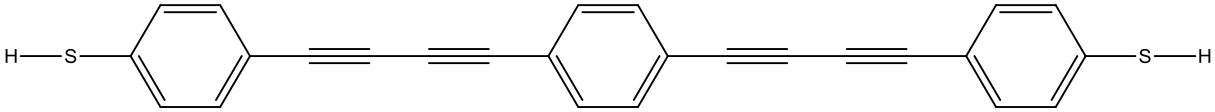
5. Thieno(2,3-bithiophene, 6. 1,2-di([1,1_-biphenyl]-4-yl)ethyne

6. 1,2-bis(4-(phenylethynyl)phenyl)ethyne

Study of 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene



(I)



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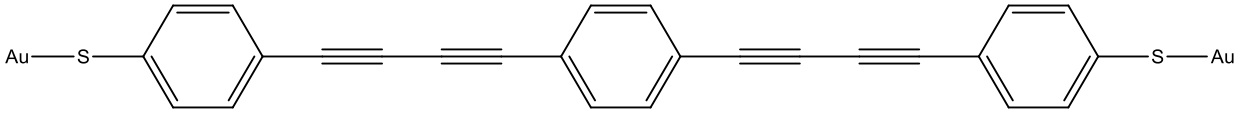


(III)

Fig.3.1 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene [(I-free molecule), (II- substituted with S) and (III- substituted with S and Au)].

4. GEOMETRICAL PARAMETERS

4.1 Bond lengths

In this chapter describes the geometrical parameters such as bond length and bond angle to analyse the structural aspects of the molecule. The geometric parameters particularly bond length is a significant parameter for adjusting the electrical properties of conducting molecules . Also, the average difference between the adjacent single and double bonds known as the bond length alternation along the backbone of a conjugated system plays a vital role for tuning the transport properties.

In the present work the bond length of (I) free molecule (II) thiol substituted molecule and (III) the molecule substituted with S and Au has been analysed for 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene molec

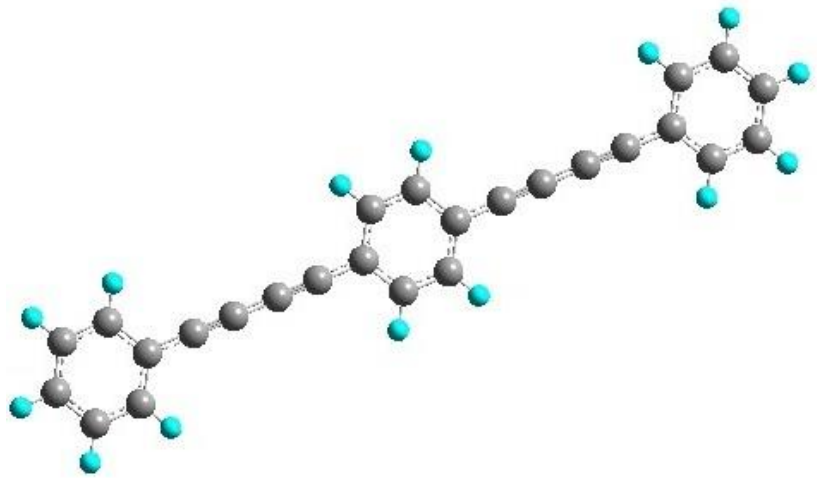
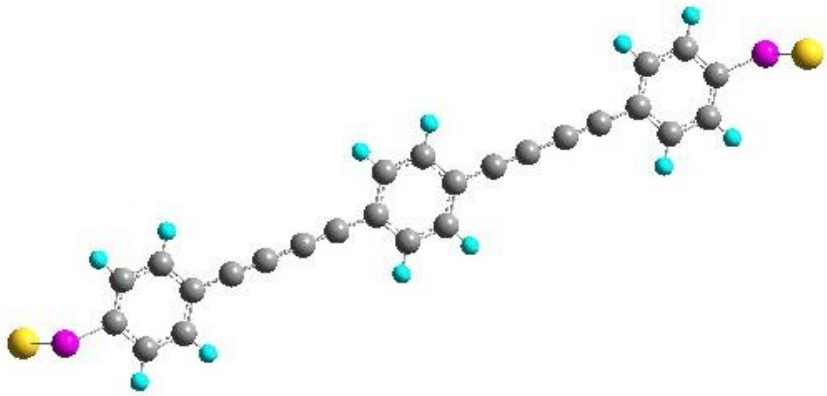
Molecule	Optimized geometry
I	
II	
III	

Fig. 4.2 Optimized geometry of 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene molecules [(I-free molecule), (II- substituted with S) and (III- substituted with S and Au)].

Therefore, a detailed study of bond length variation under the EFs interaction is instructive for understanding the relationship between molecular structure and property. Recently, the structural and electrostatic properties of numerous molecules have been studied using Density Functional Theory method. The S and Au substituted 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene molecules are shown in Fig.4.1.

The 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene molecule has been optimized and the Au atoms are attached at the ends of the molecule through S atoms. The S atom forms good link between the conjugated 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene and the Au atom. To understand the conducting property and structural stability of the molecule, it is essential to compare the free molecule with the substitution of S and Au with the free molecule . The optimized geometry of free molecule), (II-substituted with S) and (III-substituted with S and Au) is shown in Fig 4.2.

The C−C bond distances of free 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene molecule of are vary from 1.233 Å to 1.430 Å. When the molecule is substituted with S and Au, the C−C bond distances decreases to 1.428 Å; On compared with free molecule, the maximum variation observed for the molecule with S and Au are almost same value (0.003 Å) respectively. The 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene free molecule of C−H bond distances are vary from 1.086 Å to 1.087 Å. When the molecule is substituted with S and Au, these bonds are 1.088 Å and 1.086 Å respectively.

The terminal S−C bond distances of the molecule with S are found to be unequal (1.839 Å). The S−C bond distances of the molecule with Au are found to be equal 1.838 Å. The bond distances of Au−S bonds are found to be equal (2.399 Å) on both ends of the Au substituted molecule. 4.3 shows the variation of bond lengths of the molecules substituted with S and Au (II and III) with reference to the free molecule (I).

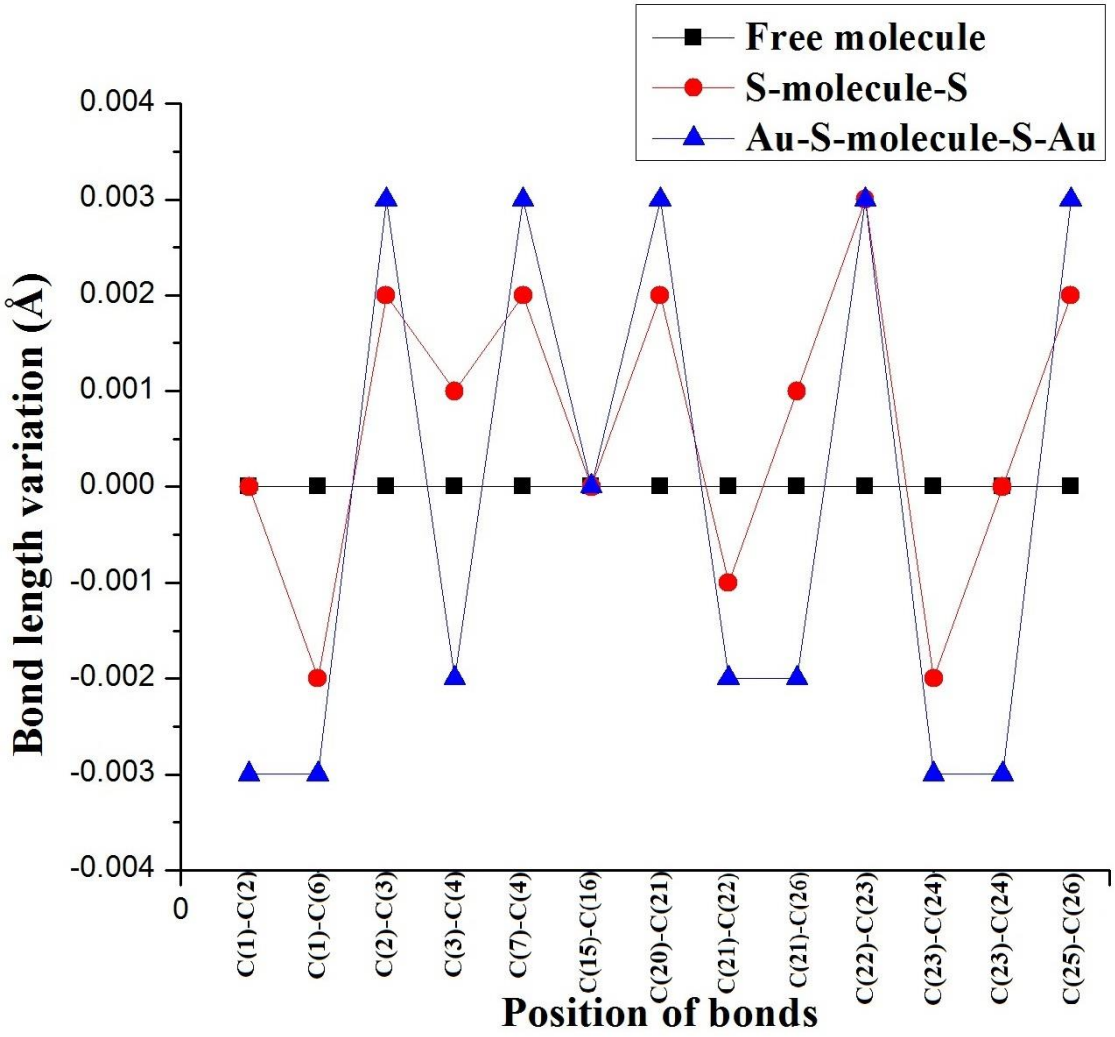


Fig. 4.3 Variation of bond lengths of the molecules substituted with S and Au with reference to the free molecule.

5. ELECTROSTATIC AND TRANSPORT PROPERTIES

5.1 Mulliken Population Analysis and Natural Population Analysis

Mulliken atomic charge calculation has a significant role in the application of quantum chemical calculation to molecular system because of atomic charges effect electronic structure, dipole moment, molecular polarizability and other properties of molecular systems . The Mulliken atomic charges are calculated by determining the electron population of each atom as defined by the basis function. Since the description of atomic populations initiated by Mulliken many alternative schemes of atomic charges have been proposed as a natural consequence of the earlier statements. In the present work, the atomic charges have been estimated from Mulliken population analysis (MPA) as well as Natural population analysis (NPA) methods for various substituted molecule.

The MPA charges of both models predict almost negative charge for all C-atoms in all the molecules-(I, II and III). The MPA charges of all C-atoms for all the four kinds of molecules vary from -0.386 e to 0.362 e. The maximum variation observed for the molecule with S and Au are 0.048 e and 0.032 e respectively. The linker atoms on either ends [S(1) and S(2)] possess same MPA charge of molecule-II are equal (-0.003 e), molecule-III are equal (0.088 e). The charges of Au atom at both ends of the molecule-III are equal -0.042 e.

The NPA charges of all C-atoms for all the four kinds of molecules vary from -0.238 e to 0.046 e. The maximum variation observed for the molecule with S and Au are 0.07 e and 0.047 e respectively. The linker atoms on either ends [S(1) and S(2)] possess same NPA charge of molecule-II are equal (0.024 e) and molecule-III are equal (-0.151 e). Similarly, the charges of Au atom at both ends of the molecule-III are equal (0.229 e). The difference of NPA charge distribution for all the molecules are listed in Table 5.2. The variations of MPA and NPA charges for the molecules-II and III with reference to molecule-I are plotted as in Fig. 5.1 & Fig.5.2.

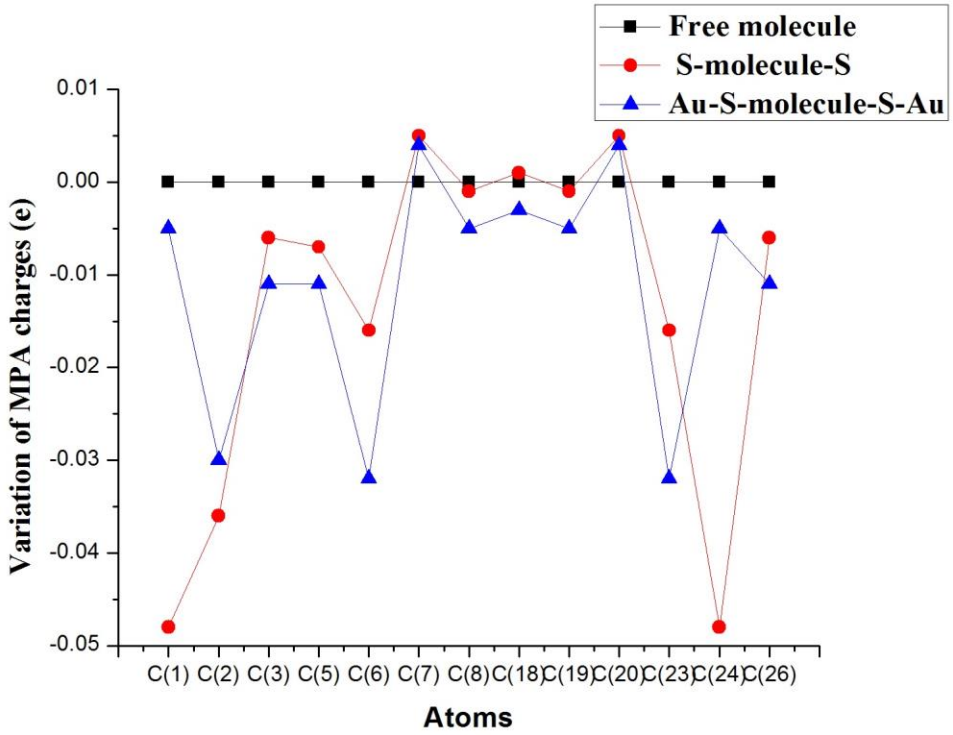


Fig. 5.1 Variation of MPA charges of the molecules-II and III with reference to molecule-I.

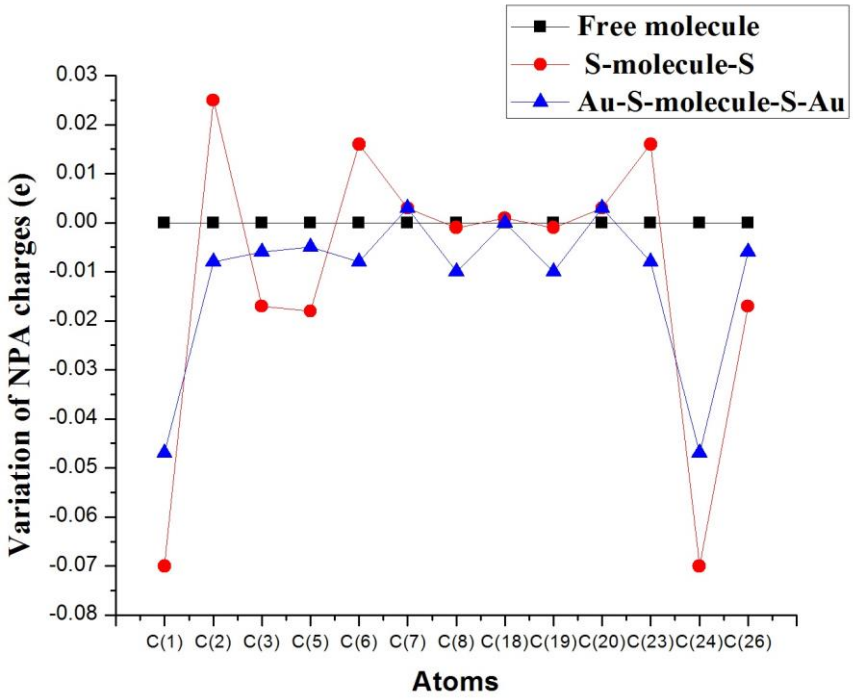


Fig. 5.2 Variation of NPA charges of the molecules-II and III with reference to molecule-I.

5.2 Molecular orbital analysis

When atoms combine to make molecules, atomic orbitals must combine to make molecular orbitals, however, the total number of orbitals does not change. Also, the orbitals must be physically close enough to interact. The magnitude of the combination is inversely proportional to the distance between the atoms. The one of the key factor in determining the electrical conductance of a molecule is HOMO-LUMO gap (HLG), which is the difference of energy between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). Hence, in this study we have analyzed the variations in HLG and molecular orbital energy levels. Fig. 5.3 illustrates the energy levels of the 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene molecule for [(I-free molecule), (II-substituted with S) and (III-substituted with S and Au)].

Fig. 5.4 [(a)-(c)], shows the density of states (DOS) for the molecules- I, II and III in which the green lines indicate the HOMO and the blue is LUMO. The HLG of molecules-I, II and III are 3.36, 3.24 and 2.11 eV respectively. The free molecule is substituted with thiol, the HLG decreases from 3.36 eV to 2.11 eV. However, it is attached with Au atoms at both ends, the HLG increases to 2.11 eV. When, the Au substituted molecule conduct the electricity. The small decrease of HLG facilitates large electron conduction through the molecule, hence, the Au substituted 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene molecule can act as an conducting molecular nanowire.

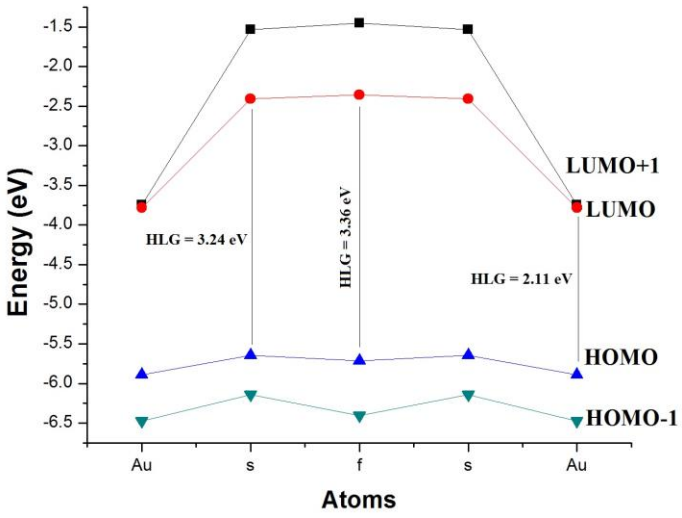
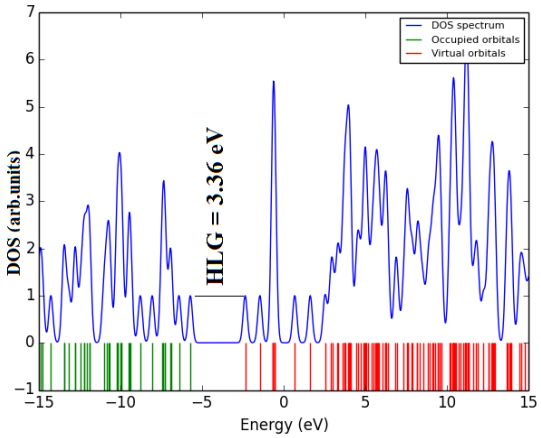
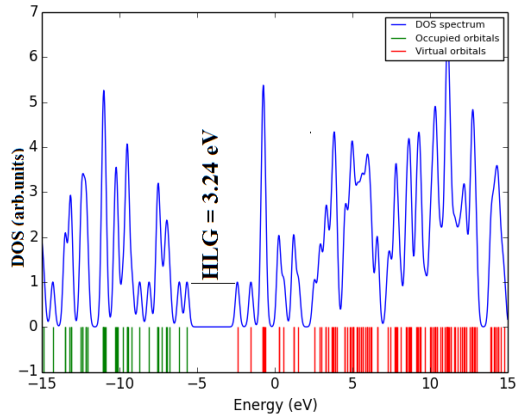


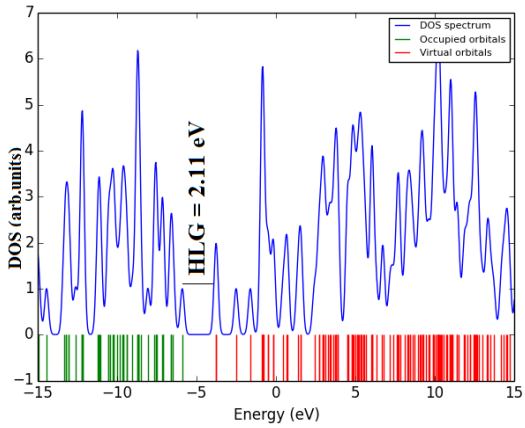
Fig. 5.3 Energy level diagram of Au and S substituted 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene molecules.



(a)



(b)



(c)

Fig. 5.4 (a-c) Shows the density of states (DOS) for the molecules-I, II and III.

SUMMARY AND CONCLUSIONS

The present research work has been carried out to study the structural, electrical characteristics and the effect of Au metal atoms on 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene molecule by computational study. The free molecule (molecule-I), S- substituted molecule (molecule-II), Au and S substituted molecule (molecule-III) have been optimized by using G09 program. A combination of Becke's three-parameter exchange function (B3LYP hybrid function) has been used for the whole calculation with LANL2DZ basis set.

The entire theoretical study on 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene molecules [(I-free molecule), (II- substituted with S) and (III- substituted with S and Au)] describes the bond structural parameters as well as the electrical characteristics. The values of bond lengths of C-H, S-C and Au-S bonds calculated from this study are almost matched with the reported results.

The MPA and NPA atomic charges shows that the atomic charges of Au atom posses negative charges, which are matched with the previous reports. The HLG of molecules-I, II and III are 3.36, 3.24 and 2.11 eV respectively. These values are compared with the values obtained from density of states spectrum (DOS). All these values are matched with the reported results. The free molecule is substituted with thiol, the HLG decreases from 3.36 eV to 3.24 eV. However, it is attached with Au atoms at both ends, the HLG increases to 2.11 eV. For thiol linked the molecule and Au substituted molecule are found to be exhibit very smaller HLG. However, the facilitates to have been electrical conductivity is very high of this molecule.

Hence, the 1,4-bis(phenylbuta-1,3-diyn-1-yl)benzene is attached to Au electrodes through thiol linker can act as good conductor. Hence, the Au substituted molecule can be used as molecular nanowire in nano devices.

Part II

1.Introduction:

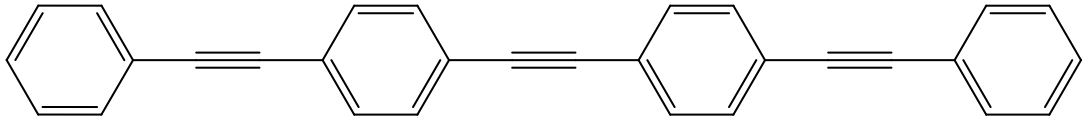
The research is carried out with the following molecules during the II year.

1. 1,2-di([1,1_-biphenyl]-4-yl)ethyne 2.dicyclopentyl-cyclohexane 3.Thiophene 4. 2,2' bithiophene 5. Thieno(2,3-bithiophene, 6. Cyclohexane

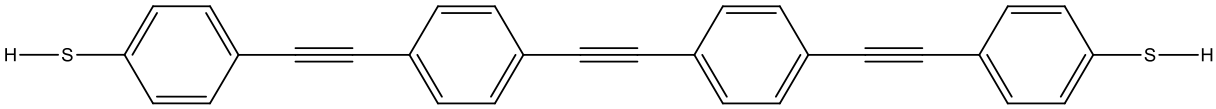
2.1. An introduction to 1,2-bis(4-(phenylethynyl)phenyl)ethyne Molecule

Molecular electronic research made a paradigm shift in miniaturization of electronic devices. Present trend in miniaturization of electronic devices suggests that, how, single molecule can be used as an electronic active element for the variety of applications. The advantage of molecules as electronic building blocks is that the molecules can be engineered to have some built in functional, such as light sensitive switches, gates or transport

elements.



(I)



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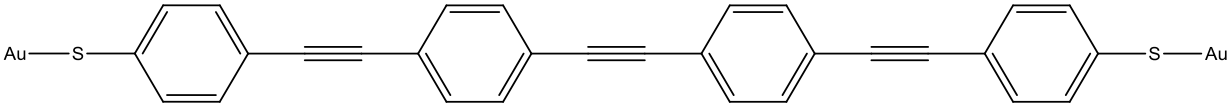


(III)

Fig. 2.1 1,2-bis(4-(phenylethynyl)phenyl)ethyne [(I-free molecule), (II- substituted with S) and (III- substituted with S and Au)].

Furthermore, recent advances show, how the single molecules can be manipulated between two electrodes and the measurement of its electronic transport properties. Imagine a wire in which the presence or absence of a single atom dominates the electrical conductivity or in which a bio-molecular recognition process is used to open up new

conductivity pathways. The π-conjugated oligomeric system provides an efficient electronic coupling between donor and acceptor termini display wire like behavior. The energy gap between the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO) of 1,2-bis(4-(phenylethynyl)phenyl)ethyne being smaller (~2eV) than the saturated molecules (~7eV), which leads to have more efficient charge transport through the molecule, hence it acts as a better molecular wire. 2.1 shows 1,2-bis(4-(phenylethynyl)phenyl)ethyne molecules [(I-free molecule), (II- substituted with S) and (III- substituted with S and Au).

3. Optimisation

In the present study, the electrical characteristics of 1,2-bis(4-(phenylethynyl)phenyl)ethyne molecular wire have been analyzed using quantum chemical calculations coupled with AIM theory.

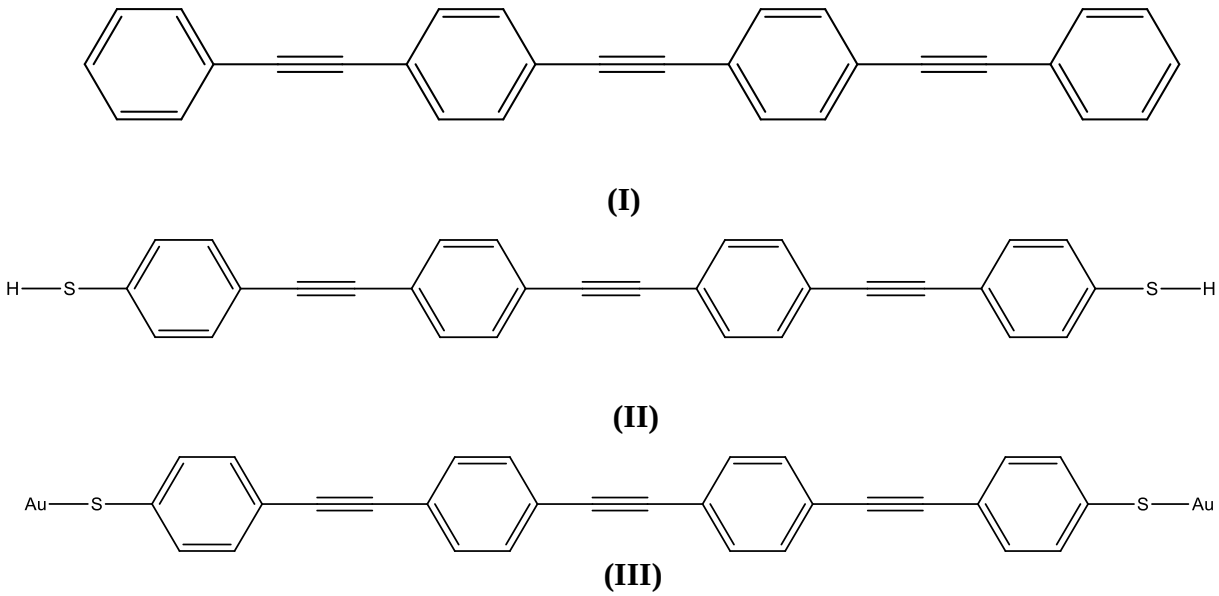


Fig. 3.1 1,2-bis(4-(phenylethynyl)phenyl)ethyne [(I-free molecule), (II- substituted withS) and (III- substituted with S and Au)].

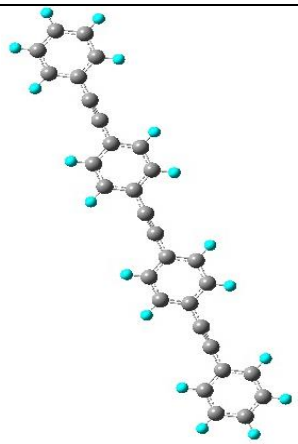
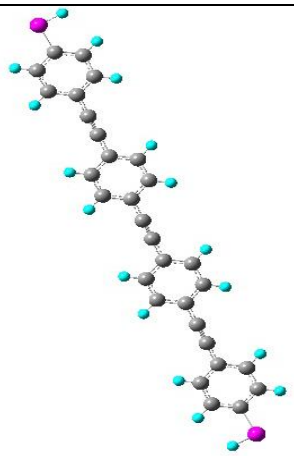
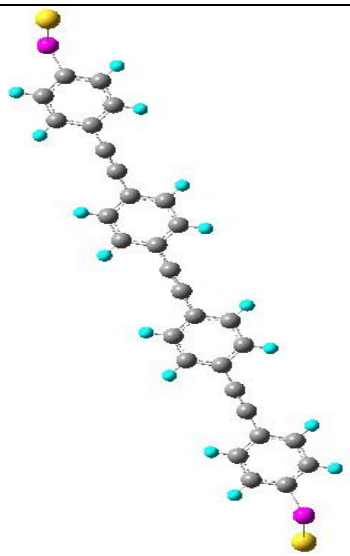
Molecule	Optimized geometry
I	
II	
III	

Fig. 3.2 Optimized geometry of 1,2-bis(4-(phenylethynyl)phenyl)ethyne molecules [(I-free molecule), (II- substituted with S) and (III- substituted with S and Au)].

Therefore, a detailed study of bond length variation under the EFs interaction is instructive for understanding the relationship between molecular structure and property. The S and Au substituted 1,2-bis(4-(phenylethynyl)phenyl)ethyne molecules are shown in Fig.3.1.

The 1,2-bis(4-(phenylethynyl)phenyl)ethyne molecule has been optimized and the Au atoms are attached at the ends of the molecule through S atoms. The S atom forms good link between the conjugated 1,2-bis(4-(phenylethynyl)phenyl)ethyne and the Au atom. To understand the conducting property and structural stability of the molecule, it is essential to compare the free molecule with the substitution of S and Au with the free molecule. The optimized geometry of free molecule), (II-substituted with S) and (III-substituted with S and Au) is shown in Fig. 3.2.

The C−C bond distances of free 1,2-bis(4-(phenylethynyl)phenyl)ethyne molecule of are vary from 1.228 Å to 1.433 Å. When the molecule is substituted with S and Au, the C−C bond distances increases to 1.430 Å; On compared with free molecule, the maximum variation observed for the molecule with S and Au are 0.003 Å and 0.004 Å respectively. The 1,2-bis(4-(phenylethynyl)phenyl)ethyne free molecule of C−H bond distances are vary from 1.087 Å to 1.088 Å. When the molecule is substituted with S and Au, these bonds are 1.087 Å and 1.086 Å respectively.

The terminal S−C bond distances of the molecule with S are found to be equal (1.840 Å). The S−C bond distances of the molecule with Au are found to be equal (1.837 Å). Similarly, the bond distances of Au−S bonds are found to be equal (2.400 Å) on both ends of the Au substituted molecule. Table. 3.1 shows bond lengths (Å) of the free molecule and the molecules substituted with S and Au. Fig. 3.3 shows the variation of bond lengths of the molecules substituted with S and Au (II and III) with reference to the free molecule (I).

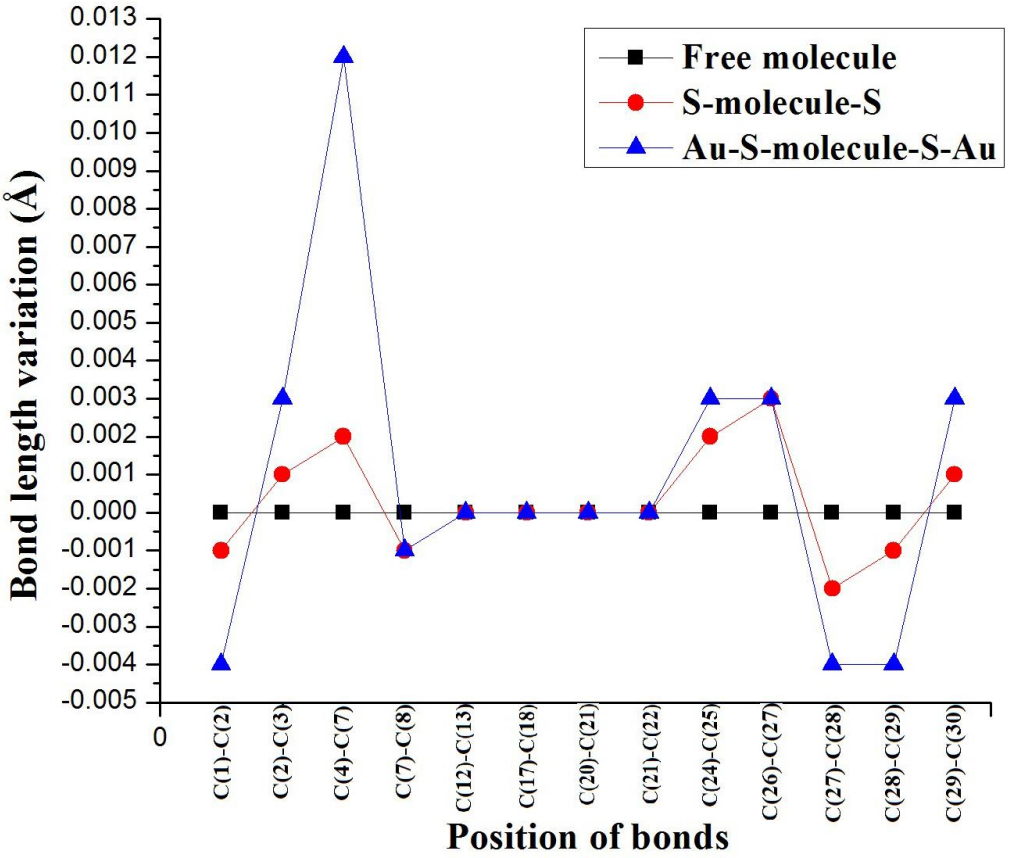


Fig. 3.3 Variation of bond lengths of the molecules substituted with S and Au with reference to the free molecule

4. ELECTROSTATIC AND TRANSPORT PROPERTIES

The MPA charges of both models predict almost negative charge for all C-atoms in all the molecules-(I, II and III). The MPA charges of all C-atoms for all the four kinds of molecules vary from -0.388 e to 0.406 e. The maximum variation observed for the molecule with S, Au and Pt are 0.052 e and 0.03 e respectively. The linker atoms on either ends [S(1) and S(2)] possess same MPA charge of molecule-II are equal (-0.007 e), molecule-III are equal (0.086 e). The charges of Au atom at both ends of the molecule-III are equal -0.049 e.

The NPA charges of all C-atoms for all the four kinds of molecules vary from -0.238 e to 0.003 e. The maximum variation observed for the molecule with S and Au are 0.073 e and and 0.049 e respectively. The linker atoms on either ends [S(1) and S(2)] possess same

NPA charge of molecule-II are equal (0.019 e), molecule-III are equal (-0.150 e). Similarly, the charges of Au atom at both ends of the molecule-III are equal (0.221 e).

The variations of MPA and NPA charges for the molecules-II and III with reference to molecule-I are plotted as in Fig. 4.1 & Fig.4.2

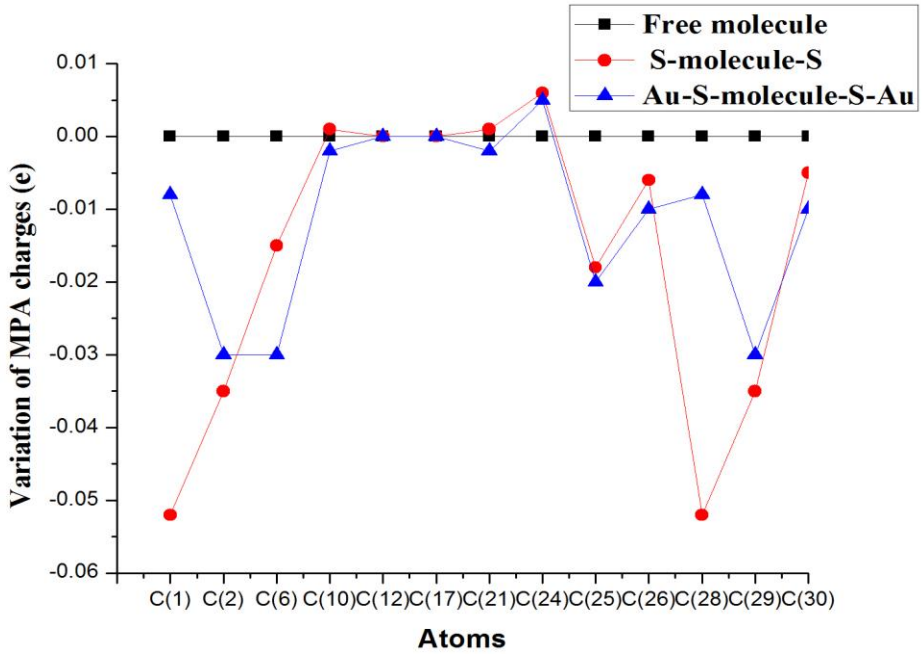


Fig. 4.1 Variation of MPA charges of the molecules-II and III with reference to molecule-I.

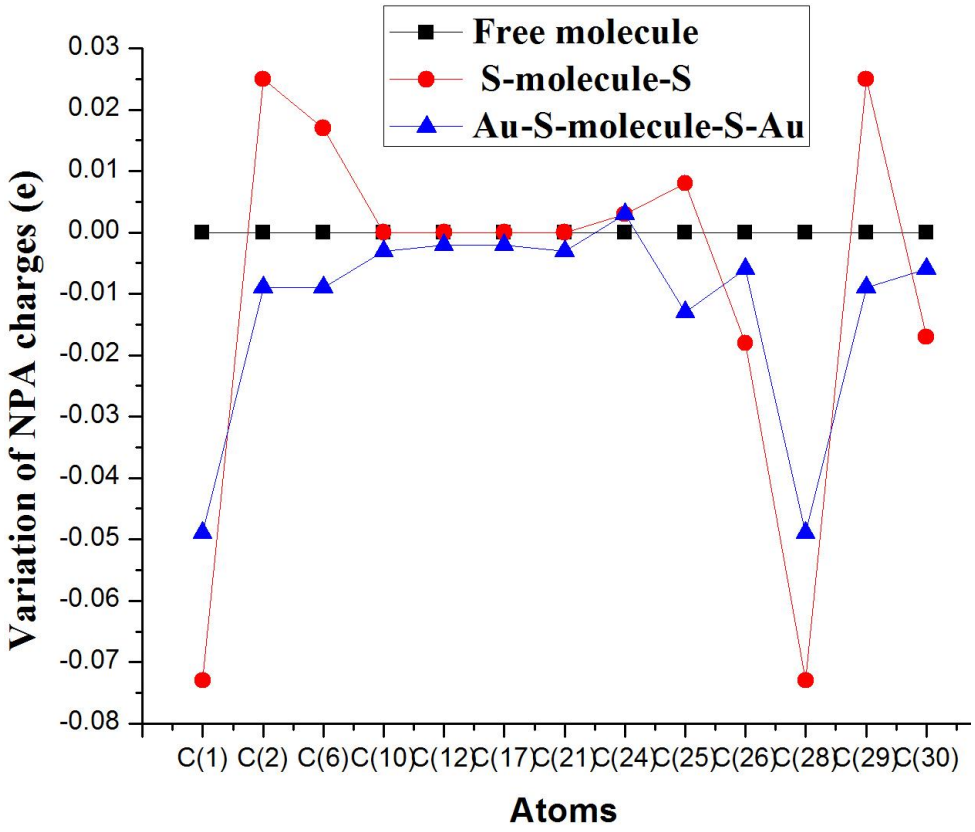


Fig. 4.2 Variation of NPA charges of the molecules-II and III with reference to molecule-I.

4.2 Molecular orbital analysis

Fig. 4.3 illustrates the energy levels of the 1,2-bis(4-(phenylethynyl)phenyl)ethyne molecule for [(I-free molecule), (II-substituted with S) and (III-substituted with S and Au)].

Fig. 4.4 [(a)-(c)], shows the density of states (DOS) for the molecules- I, II and III in which the green lines indicate the HOMO and the blue is LUMO. Here, the hybridization of the molecular level with that of the gold atom broadens the DOS peaks.The HLG of molecules-I, II and III are 3.40, 3.31 and 2.06 eV respectively. The free molecule is substituted with thiol, the HLG decreases from 3.40 eV to 3.31 eV. However, it is attached with Au atoms at both ends, the HLG increases to 2.06 eV. For both positive as well as negative bias, the energy level variations of the molecule are almost symmetric and hence the conductivity of the molecule is irrespective of the direction of external electric field. The large decrease of HLG of the molecule-III facilitates large electron conduction through the

molecule, hence, the Au substituted 1,2-bis(4-(phenylethynyl)phenyl)ethyne molecule can act as an efficient molecular nanowire.

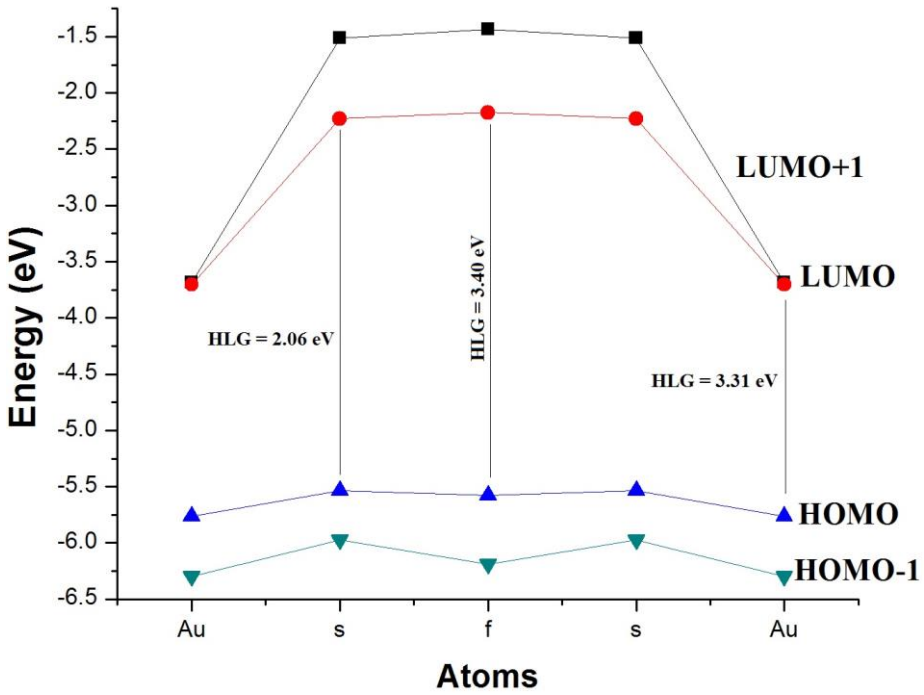
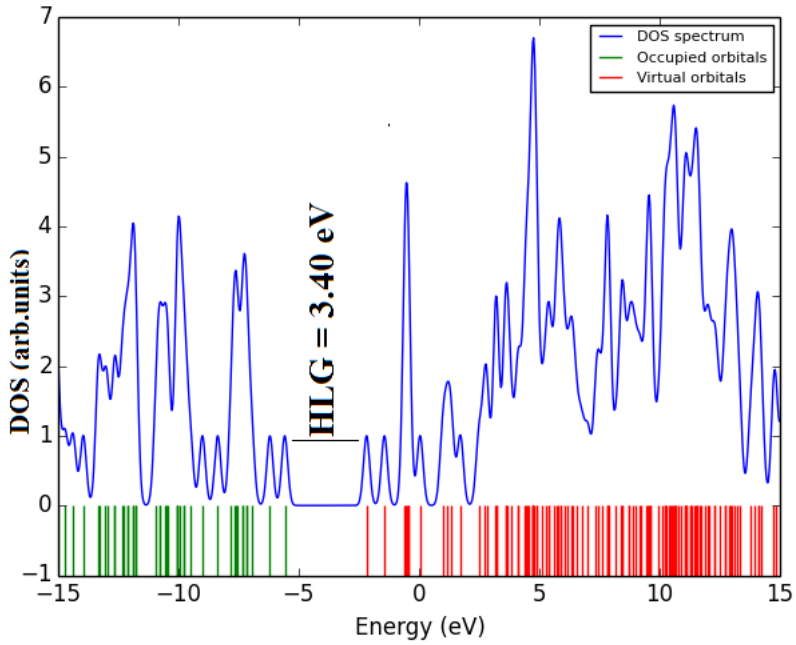
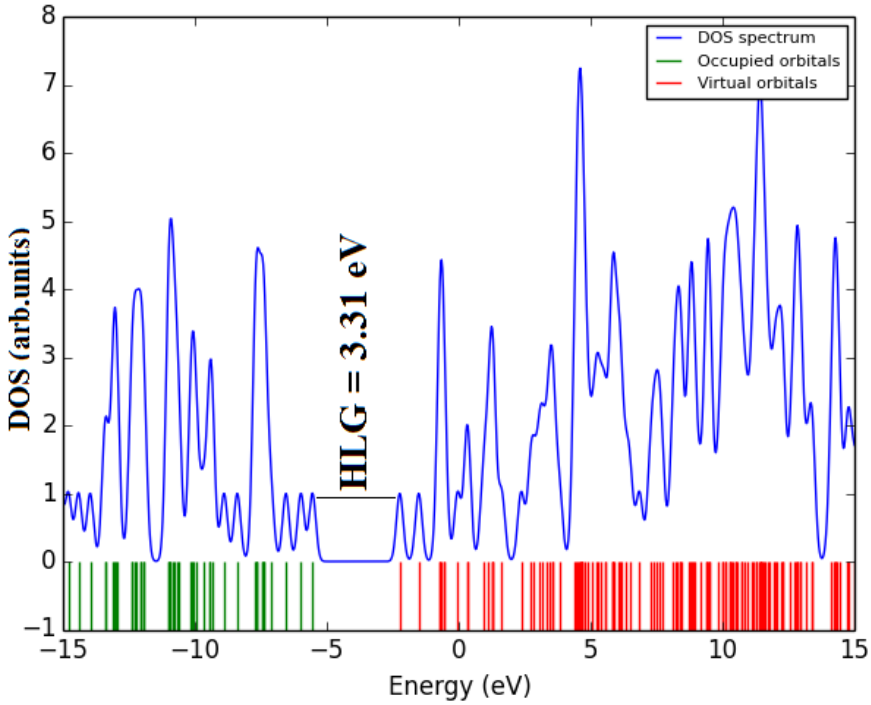


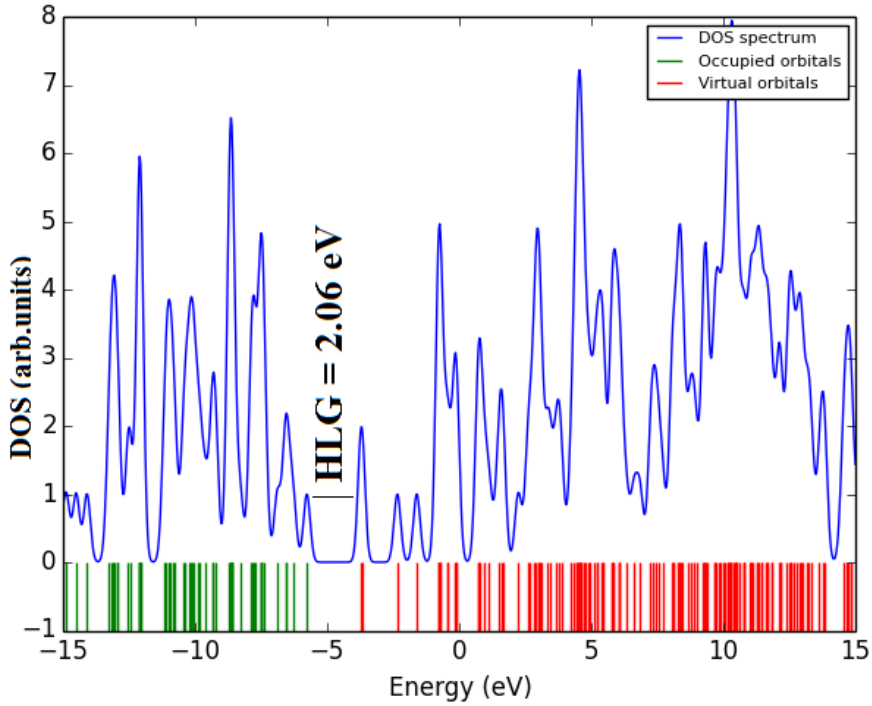
Fig. 4.3 Energy level diagram of Au and S substituted 1,bis(4(phenylethynyl)phenyl)ethyne molecules.



(a)



(b)



(c)

Fig. 4.4 (a-c) Shows the density of states (DOS) for the molecules-I, II and III.

SUMMARY AND CONCLUSIONS

The present research work has been carried out to study the structured, electrical characteristics and effect of Au metal atoms on 1,2-bis(4-(phenylethynyl)phenyl)ethyne molecule by computational study. The free molecule (molecule-I), S- substituted molecule (molecule-II), Au and S substituted molecule (molecule-III) have been optimized by using G09 program. A combination of Becke's three-parameter exchange function (B3LYP hybrid function) has been used for the whole calculation with LANL2DZ basis set.

The entire theoretical study on 1,2-bis(4-(phenylethynyl)phenyl)ethyne molecules [(I-free molecule), (II- substituted with S) and (III- substituted with S and Au)] describes the bond structural parameters as well as the electrical characteristics. The values of bond lengths of S-C and Au-S bonds calculated from this study are almost matched with the reported results.

The MPA and NPA atomic charges shows that the atomic charges of Au atom posses negative charges, which are matched with the previous reports. The HLG of molecules-I, II and III are 3.40 eV, 3.31 eV and 2.06 eV respectively. These values are compared with the values obtained from density of states spectrum (DOS). All these values are matched with the reported results. The free molecule is substituted with thiol, the HLG decreases from 3.40 eV to 3.31 eV. However, it is attached with Au atoms at both ends, the HLG decreases to 2.06 eV. But, Au metal electrodes are user friendly and low cost comparing with Pt metal. Hence, the Au substituted 1,2-bis(4-(phenylethynyl)phenyl)ethyne molecule can act as an efficient molecular nanowire.

Further, these molecules can be used as conducting wires in molecular electronic devices. This study may be useful to synthesize conducting layers and to study the effect of Au metal electrodes associated with various organic molecules.

This Minor Research Project definitely helps to design new conducting conjugated chain organic molecules with number of aromatic rings and thiophene rings which will be very useful in Nano Devices.

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