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Observation of Terminal Atom Effect on Charge in NH_2-Cn-NO_2 Molecule: A Hartree- Fock Theory

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ABSTRACT
Observation of terminal atom effect in molecule NH_2-Cn-NO_2 placed between gold electrodes with end atom sulfur and hydrogen studied using Hartree- Fock theory method. The conductance in molecule exponentially decreases with increases in the number of carbon connectors. Observed that the coupling between the molecule and the two electrodes and the energy gap between the highest occupied molecular orbital and the lowest unoccupied molecular orbital of the molecule dominate the transport property of the current.

Keywords
HLG, Muliken Charge, Molecular diode

1. INTRODUCTION
SILICON-BASED integrated circuits have experienced phenomenal growth since the invention and demonstration of the earliest devices: the first bipolar transistor in 1948, the first planar integrated circuit in 1961 and the first general purpose metal–oxide–semiconductor field-effect transistor (MOSFET) in 1964. Today the semiconductor industry has combined revenues of over 200 billion dollars and its technical progress is typical example by main products listed as: microprocessors operating at 1 GHz or more [1]–[5], microprocessors with 100 million transistors [4] and [5], and memory chips with 1 GB densities [6]–[9]. This rapid technological progress was first predicted in 1965 by Gordon Moore in the now famous "Moore's Law" which stated that integrated circuit density and performance would double every 18 months. These improvements would come from reduced transistor dimensions, increased transistor numbers, and increased working frequencies. His forecast was remarkably prophetic.

Silicon-based technology will eventually run into main limits and not be able to provide the expected increases in density and performance. Evolutionary technology improvements that have been the foundation of integrated circuit development for the past 50 years. A new and revolutionary integrated circuit technology [12] will be needed to replace MOS transistors as the driver behind continued improvements in electronic products. Some new types of nanotechnology devices are interesting candidates to explore, but the success of silicon MOS transistors will be hard to replace. It took many years for bipolar and MOS transistors to make the transition from laboratory devices to useful products. A serious effort by academic and industrial researchers is needed now to explore nanotechnology options as possible replacements for MOS transistors, whose scaling limit may not be that far away.

Recently, many experimental and theoretical works carried out the transport properties through single molecules, or even the design of molecular electronic devices. However, before practical molecular electronic devices can be fabricated, more profound understanding of the transport process through such single molecular devices.

2. METHODOLOGY & SIMULATION SETUP
The calculations were carried out recently developed Argus lab package [11-14]. The package is based on the combination of Extended Huckel theory, Hartree Fock theory calculations, molecule surface visualization, calculation of U/V visible absorption, and calculate single-point energy of molecule. The setup used for all the models 2H, 2S,3H and 3S sets of simulations is shown in figure 1. The study of electronic transport properties through the molecule device, take an Extended Huckel description. More specifically, construct the extended molecule, including a gold atom between the molecules, as suggested by Lang et al. The extended molecule is studied by the self-consistent Hatree Fock (HF) method using the LANL2DZ, with effective core potential of the gold atoms. The two gold electrodes are described by a standard tight-binding parameterization for bulk elemental solids. The conductance through the whole device is calculated by using a Green's functional technique [16].

The external potential bias taken part in the self-consistent calculation directly. Therefore the effects of the bias voltage on the electron structure of the system can be fully considered. Detailed of the method and relevant references can be obtained elsewhere [10-13]. In our calculations the convergence criterion for the Hamiltonian, charge density and band structure, energy is [10] and the atomic cores are described by norm conserving pseudo potentials.

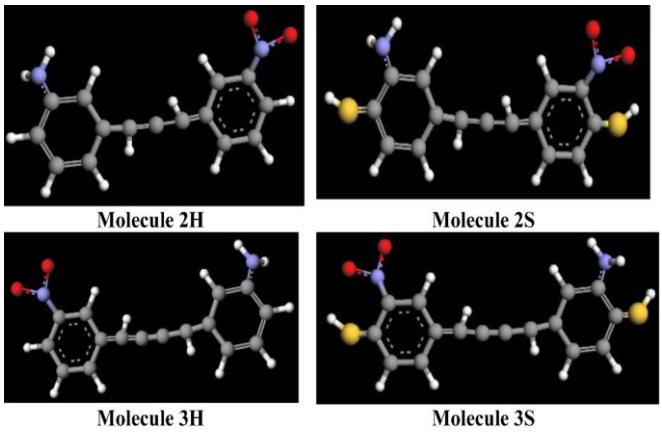

Fig. 1: The Molecular Structures under Study with and without Sulfur Atoms

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3. RESULTS AND DISCUSSIONS

Firstly the equilibrium conductance as a function of the number n of CH2 has been studied and is shown in fig 2. Investigated that increase of n the conductance decreases exponentially in the molecular wire. The conductance is 0.14G0 (G0=$2e^2/h$, quantum conductance) for n=0, 0.04G0 for n=1, 0.009G0 for n=3 soon. The exponential decrease of conductance with the length increase of carbon chains has been identified in other literature papers[16-19].

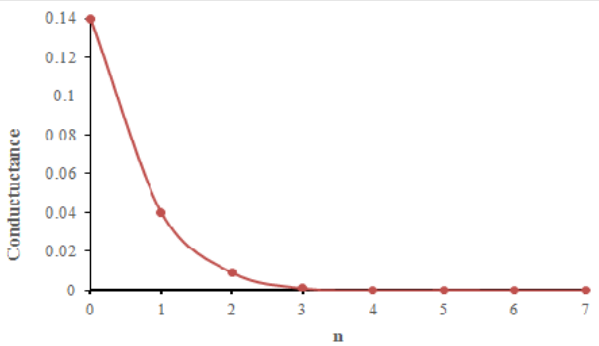
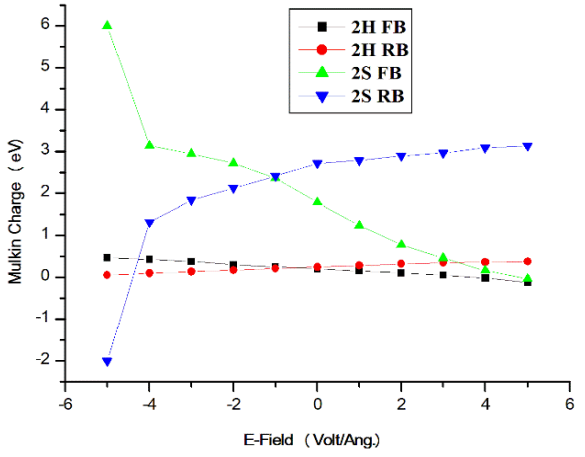
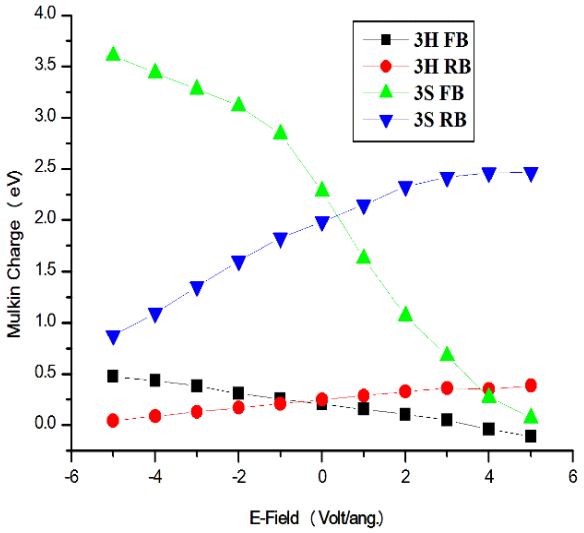


Fig. 2: The Conductance in terms of n

In this research paper, NH2 molecule act as donor particle donating the electron under electric field applied, and NO2 act as acceptor particle, accepting electrons injected in the positive bias side. Based on the π- orbital theory, the behavior of molecules 2H and 2S totally unlikely. 2H connected end point hydrogen atom connected to gold atoms, and 2S connected with the sulfur atoms connected to gold atoms, same as 3H and 3S also only change in the acceptor and donor molecules connection with the three carbon chain. Apply the electric field to 2H, 2S, 3H and 3S molecules from 0 Volt/Ang. to 5 Volt/Ang. Using Argus Lab [14] observed HOMO and LUMO gap (HLG), observation of HLG of molecules 2H much larger than that of molecule 2S. It is also seen that the HOMO and LUMO of molecule 2S have been expanded into a continuous distribution of orbital energy, while the observation of 3S one side of the molecule only, no orbital distribution at the other side. As a result two factors will involve roles in the transport process, the coupling between the molecule and the two electrodes. The larger the coupling and smaller HLG and the larger density of states between HOMO and LUMO and then larger conductance observed.



(a)



(b)

Fig. 3: The E-field and Muliken charge curves for (a) n=2 with and with sulfur connector (b) n=3 with and without sulfur atom

As pointed above, the electrical conduction properties of molecules are dominated by the variation of its HLG. In our study E-field applied from -5 volt/Ang. to 5 Volt/Ang. for both forward bias and reverse bias charge formation plotted see in figure 3 (a) and 3 (b). From Fig 3 (a) connector molecule hydrogen atom charge formation for both forward bias and reverse bias voltages almost maintain a linear value, variation of charge -0.0202 eV to 0.4685 eV and its very small, but whenever sulfur atom connectors are used charge formation increased from -0.0399 eV to 6.0016 eV. In forward bias as a voltage increases Muliken charge formation deceases vice versa. The same analogy applied to the when molecules connected with 3 number of carbon atoms.

4. CONCLUSION

We have investigated conductance of molecular wire charge formation increases on acceptor side and donor side when the sulfur atom connected. Molecule connectors even number of SP orbital chains are connected its act like a conducting wire observed using HLG, if connected using an odd number of SP orbital act like a molecular diode, observed using the Argus Lab software. The period of the conductance is determined by the filling factor of the conduction band of the Sulfur atoms with specific interaction spacing.

5. ACKNOWLEDGEMENT

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