Single Molecular Transistor

A Thesis

Submitted to the Department of Electrical and Electronic Engineering

Of

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In partial fulfillment of the requirements for the degree of

Bachelor of Science in Electrical and Electronic Engineering

Fall 2017

BRAC University, Dhaka

Declaration

We therefore proclaim that proposition work titled “Single Molecular Transistor” is our own work. The work has not been introduced somewhere else for evaluation. Where materials utilized from different sources have been legitimately recognized and alluded.

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Date of Submission: Dec 26, 2017

Acknowledgement

Initially, we would like to express gratitude toward Md. Anamul Hoque, Lecturer, Dept. of Electrical and Electronic Engineering (EEE), BRAC University; for his encouraging instruction and contribution for the accomplishment of this thesis. Also, our appreciation is towards BRAC University for subsidizing this thesis and making it worthwhile.

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Abstract

Electron transport through single particles is emphatically influenced by single-electron charging and the vitality level quantization. In this proposition, we research electron transport in single particle transistors made with a few unique particles, including fullerene particles and single Co particles with various lengths. To perform transport estimations on these little (<3 nm) particles, cathodes with a hole that is 1~2 nm wide are manufactured using the electro migration-intersection system. We likewise considered single-walled carbon nanotube gadgets that are manufactured utilizing a more customary strategy.

At low temperatures, most single atom gadgets show Coulomb blockade with discrete conductance tops that relate to quantum excitations of the atom. The cause of the watched quantum excitation changes from atom to particle contingent upon how burrowing electrons collaborate with different sub-atomic degrees of opportunity. Vibration excitation is the one that is most much of the time watched. The most conspicuous vibration excitation was recognized as the skipping ball mode in C60 and C70 transistors, though it was allotted to the interchange extending mode in C140 transistors. Attractive excitation was additionally considered, and the turn condition of a solitary Co particle was dictated by breaking down the Zeeman part in an attractive field.

The general conductance of single particle transistors is resolved predominantly by the coupling with anodes. In single Co transistors, the coupling could be controlled by changing the length of protecting handles. With a more drawn out handle, the

conductance is lower as the single Co shapes a quantum dab. With a shorter handle, the coupling amongst Co and cathodes and also the general conductance turns out to be huge and the Kondo impact was watched.

Finally, the conductance of carbon nanotubes was examined in two extraordinary temperature administrations. At low temperatures, they shape a solitary quantum dab (p-doped) or a twofold quantum dab (n-doped) because of a nearby doping by the cathodes. In room temperature estimations, a profoundly proficient electrolyte door was utilized to explore the field impact transistor properties of carbon nanotubes, which revealed phenomenal gadget exhibitions.

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Chapter 1

Molecular electronics is the field of science that researches the electronic and thermal transport properties of circuits in which singular molecule (or a gathering of them) are utilized as essential building blocks [2]. With a specific end goal to plan and acknowledge single-molecule devices it is basic to have a decent comprehension of the properties of a single molecule. For electronic applications, the most critical property of a particle is its conductance. In view of this learning we have acknowledged one single-molecule device: a single molecule transistor. Through mechanical gating, i.e., compacting or extending of the octanethiol molecule, by varying the contacts interspaced, we can efficiently modify the conductance of the electrode octanethiol-terminal intersection. This two-terminal single-molecule transistor is extremely powerful, yet the enhancement factor is somewhat constrained [4].

1.1 Introduction to the Single molecular transistor

The utilization of a gate electrode enables us to increase further understanding into the electronic structure of atomic intersections. It is broadly utilized for spectroscopy of the atomic levels and its energized states, for changing the charge condition of the particle and exploring higher request procedures, for example, co-tunneling and the Kondo impact. Gate terminals have been executed in a few sorts of nanoscale gadgets, for example, electron migration intersections, mechanically controllable break intersections, and devices with carbon-based electrodes. Here we audit the cutting edge in the field of single-molecule transistors. We examine the test challenges and portray the advances made for the distinctive methodologies [3].

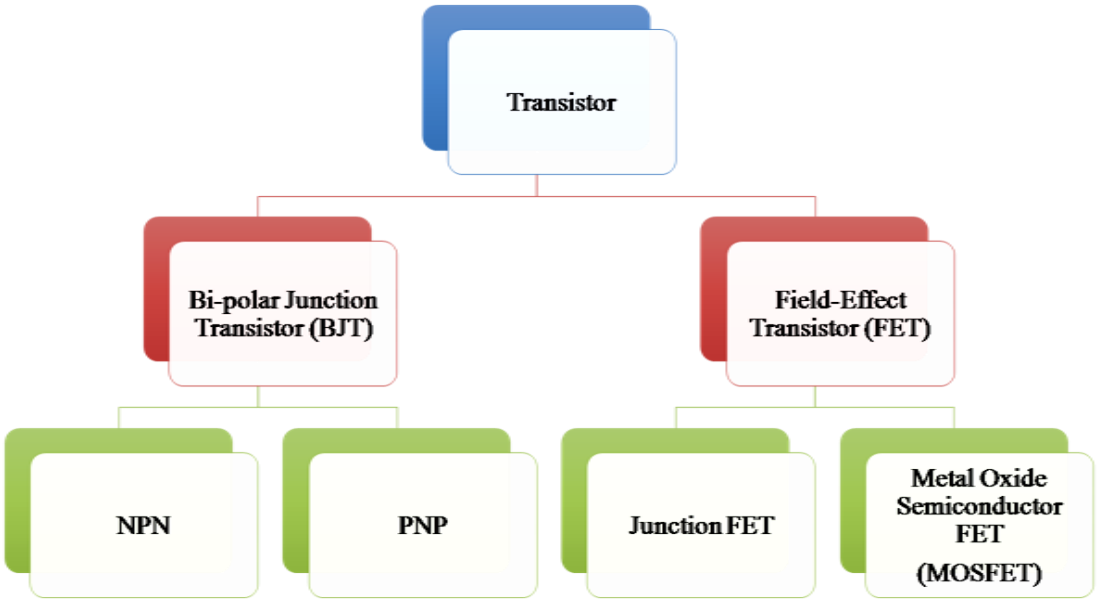


Fig 1.1 Classification of Transistor

1.2 What is MOSFET & current trends of MOSFET

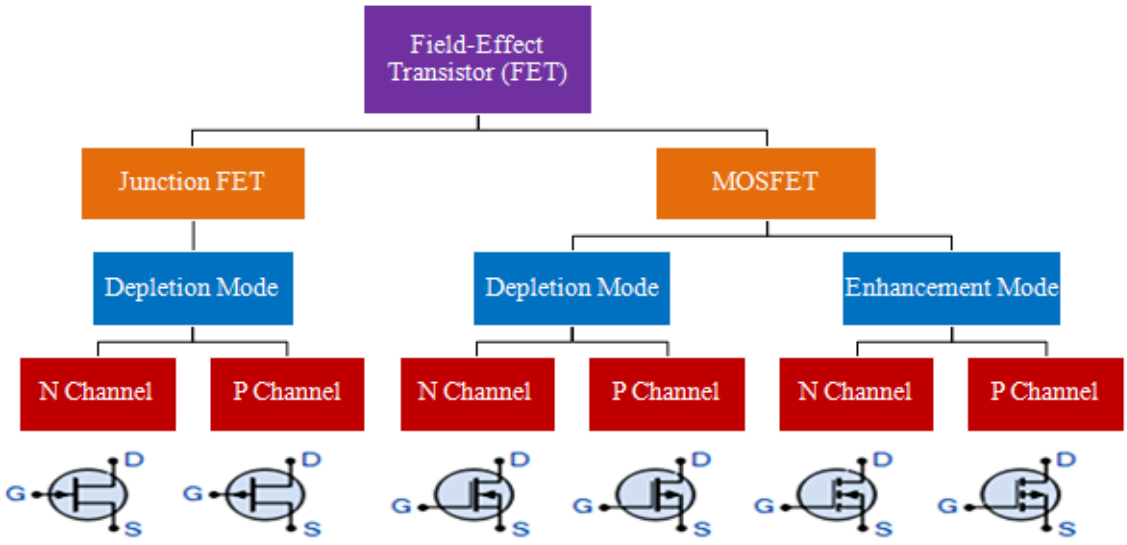


Fig 1.2.1 Classification & Simplified Configuration of FET

A metal– oxide– semiconductor field-effect transistor (MOSFET, MOS-FET, or MOS FET) is a field-effect transistor (FET with an insulated gate) where the voltage decides the conductivity of the device. It is utilized for exchanging or enhancing signals. The capacity to change conductivity with the measure of connected voltage can be utilized for intensifying or exchanging electronic signs. Nowadays MOSFETs are significantly more typical than BJTs (bipolar junction transistors) in both analog and digital circuits.

It is past anybody's creative energy in the matter of how the MOSFET (Metal-Oxide Semiconductor Field-Effect Transistor) could have advanced in the previous 40 years, Moreover, it is likely that 10 years from now we won't be able to perceive a MOSFET as it is today. Even though a few intellectuals have anticipated that the advancement of semiconductor innovation to littler measurements will back off as the component estimate hit the 0.1−μm stamp, the improvements in certainty have been accelerating as of late.

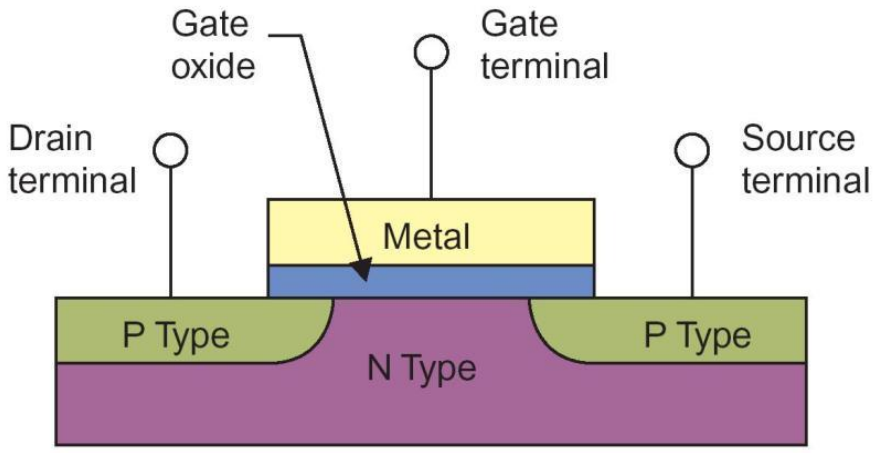


Fig 1.2.2 MOSFET (simplified configuration)

The ITRS (International Technology Roadmap for Semiconductors) as of late changed its projection for the 2003 innovation hub from 120 nm (ITRS 1999 issue) to 100 nm (ITRS 2001, 2002 updated), and the focused on gate length for MOSFETs in elite rationale circuits for 2003 from 85 nm (ITRS 1999) to 45 nm (ITRS 2001).

Consistent MOSFET scaling and synchronous increment of chip estimate prompted increasingly complex incorporated rationale circuits with improved speed and execution. For instance, chip produced by Intel Corp. have seen the quantity of transistors per chip increments from 2300 out of 1971 (Intel 4004) to more than 108 out of 2003, as showed in Fig. 1.2. The clock recurrence of the processors, then again, has been expanded from 1 MHz in 1971 (Intel 4004) to around 3 GHz in mid-2003 (Pentium 4) [1].

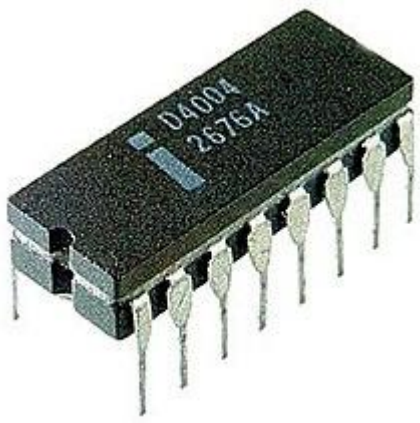


Fig 1.2.3 Intel 4004

1.3 Motivation

Benefits of single molecular transistor and its uses are the key to the motivation of exploring and investigating the whole molecular electronics field. Molecular electronics as well as single molecular transistors have benefits of lesser manufacturing complexity, easier scaling and less power consumption as well [5]. Molecular electronics such as molecular transistor offers, as an example, the chances to explore and invent thermal as well as electronic conduction in a smaller possible scale [2]. Electrical conduction using molecules relies basically on the de-localization of the molecule's electronic orbital and their association with the metallic contacts [6,7]. The application of molecule transistor is key components in future nano-electronics and the basic enthusiasm of comprehension the microscopic transport through a solitary or little gathering of molecules [9]. Till now, most break junction estimations have been done in arrangement utilizing scanning probe devices. Despite the fact that this gives off an impression of being an exceptionally appropriate condition for concentrate single-molecule references, it additionally forces a critical farthest point on the analyses: the temperature extend is confined to a couple of tens degrees [10].

Mechanically controllable break intersections (MCBJs) don't experience the ill effects of this confinement. They can without much of a stretch be worked down to cryogenic temperatures in a vacuum situation. Besides, the electrode separation in these tools displays outstanding dependability over the whole temperature range [11].

1.4 Challenges & limitation

As every invention single molecule transistor faces various summonses as well. The significant test in this field is interfacing nanometer-scale objects (particles) with naturally visible circuits. The extent of natural molecules is in the scope of 1-10nm, subsequently no less than two plainly visible metallic terminals isolated by a similar separation are required for the most essential, by and by the most principal electrical estimations. Controlled manufacture in this length scale is past the extent of most present day lithographic strategies [9]. For instance, a gate electrode is needed to be added to a mechanically-controllable break-junction (MCBJ), for mechanical adjustability and combining electrostatic gating. MCBJ comprises of a restricted extension of metal suspended over an adaptable substrate, and bending of the substrate can break the bridge which eventually adjusts spacing between resulting electrodes. Challenge faced in fabricating this electrically-gated MCBJ is mainly while minimizing the molecule-gate space in order to enable useful gating [8]. The MCBJ and Scanning probe microscope are two of the all other techniques used for studying the microscopic transport through molecules. These two techniques in general hold lacking of electrical and mechanical stability which is required for transport measurements below dissimilar ambient conditions [9].

1.5 Project overview

- The overall discussion about the electronic properties as well as the transportation system of single molecule transistor is mentioned in this dissertation.

- Fabrication procedures and its uses are also briefly mentioned here.

- Simulation results and summarized discussion on the equations pertaining to the single molecule transistor is also referred here.

1.6 Summary of the following chapters

In the following chapters the above mentioned features are discussed thoroughly. Chapter 2 is on the transportation system of electron in a single molecule device, e.g. transistor. Single electron transistor is an almost alike molecular device as single molecule transistor, features and overall theory of which is also mentioned in chapter 2. Some examples of single molecule devices and along with that, single molecular charging energy and excitation spectrum is mentioned there. Coulomb blockade is another highly related and important phenomenon regarding single molecule devices, which is briefly discussed in chapter 3. By relating to coulomb blockade theory, the basic concepts of single electron transistor are mentioned there. Lastly equations pertaining to single molecule transistor are stated and described, as well as summarized in chapter 5. The related graphs and results of those mentioned equations are discussed in the last chapter.

Chapter 2

A mix of established Coulomb charging, electronic level spacing, turn, and vibration modes decides the single-electron transfer responses through nanoscale frameworks associated with outer anodes by burrowing obstructions [54].Molecular conductance intersections are structures in which single molecules or little gatherings of molecules direct electrical current between two anodes. In such junctions, the association between the molecule and the electrodes incredibly influences the I-V characteristics [7].

2.1 Electron-transport in a single molecule device

One of definitive objectives in nanotechnology is building an electronic device utilizing singular molecules. To accomplish this it will be important to quantify, control and comprehend electron transport through molecules connected to electrodes. Electron transport through the molecule might be controlled mechanically, electrically, optically, magnetically synthetically and electrochemically, prompting different potential device applications. To achieve a definitive objective in device applications, trial systems to create such an electrode– molecule– electrode junction, and hypothetical strategies to portray the electron transport properties must be produced. Both are testing errands, however quick advances have been made as of late [55].

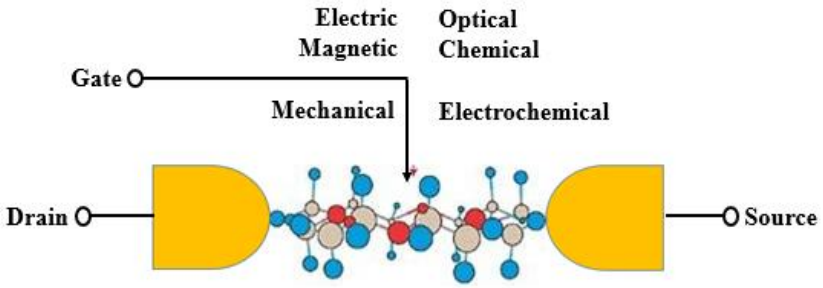


Fig 2.1.1 Illustration of a single molecule attached to two electrodes as a basic component in molecular electronics

2.2 Single electron transistor theory

Device applications require molecules to work like a wire as well as a dynamic component that can perform one or an arrangement of controllable capacities. Silicon-construct devices depends fundamentally with respect to three-terminal devices, for example, transistors. A diode or rectifier is an essential electronic tool which lets electric current for flowing in one direction by blocking in other direction. This is also an important element in making a transistor. The single-molecule diode works just as mentioned and described in fig 2.2.1. The figure shows, by using a mechanically controlled break-junction method, one molecule which consists of two weakly coupled conjugated units [55].

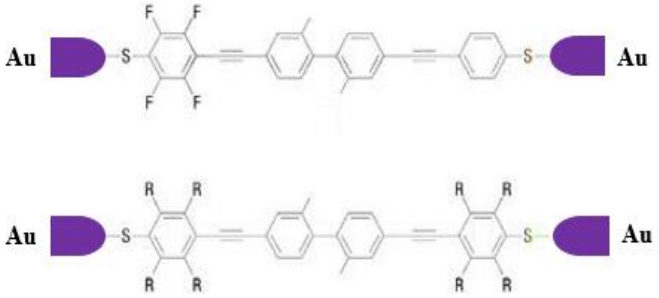


Fig 2.2.1 A molecular diode consisting of a single molecule covalently linked to two Au electrodes of a MCBJ

Three terminal devices are highly desired than two terminal devices (diodes), as the modulation of conductance is possible of a single molecule with one gate electrode alike the regular FET. The simplified configuration shown here has allowed researchers to investigate different phenomena in single molecules or a lesser number of molecules, but the needs for highly qualified fabrication facilities as well as low yield have not allowed it to be a regular technique to be used. These gate single-molecule transistors are till now widely in the single-electron transistor regime.

2.3 Examples of single molecule devices

Normal for molecules utilized as a part of single-molecule devices is that the structures contain many substituting twofold and single bonds (see additionally Conjugated framework). This is done on the grounds that such examples delocalize the molecular orbital, making it feasible for electrons to move unreservedly finished the conjugated territory.

Transistors:

Single-molecule transistors are in a general sense not quite the same as the ones known from mass devices. The gate in an ordinary (field-impact) transistor decides the conductance between the sources and deplete terminal by controlling the thickness of charge bearers between them, though the gate in a single-molecule transistor controls the likelihood of a solitary electron to hop on and off the molecule by changing the vitality of the molecular orbital. One of the impacts of this distinction is that the single-molecule transistor is relatively binary: it is either on or off. This contradicts its mass partners, which have quadratic reactions to gate voltage.

Fig 2.4.1 is a STM image of a phthalocyanine molecule centered within a hexagon assembled from twelve indium atoms on an indium arsenide surface. The positively charged atoms provide the electrostatic gate of the single-molecule transistor [Credit: PDI].

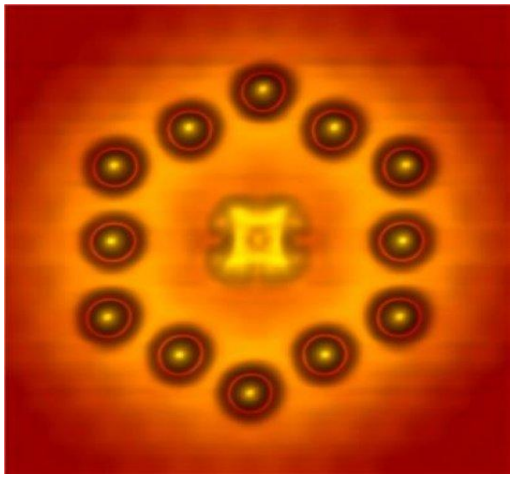


Fig 2.4.1

Wires:

The sole reason for molecular wires is to electrically associate distinctive parts of a molecular electrical circuit. As the get together of these and their association with a naturally visible circuit is as yet not aced, the concentration of research in single-molecule devices is fundamentally on the functionalized

molecules: molecular wires are portrayed by containing no utilitarian gatherings and are henceforth made out of plain reiterations of a conjugated building block. Among these are the carbon nano-tubes that are very huge contrasted with alternate proposals however have indicated extremely encouraging electrical properties.

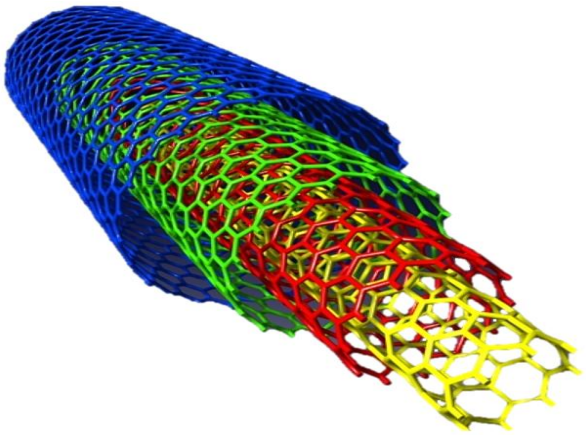


Fig 2.4.2 Carbon nanotube

Rectifiers (Diodes):

Molecular rectifiers or diodes are emulates of their mass partners and have a lopsided development with the goal that the molecule can accept electrons in a single end yet not the other. The molecules have an electron donor (D) in one end and an electron acceptor (A) in the other. The outcome is that an electric current can be drawn through the molecule if the electrons are included through the acceptor end, however less effectively if the invert is endeavored.

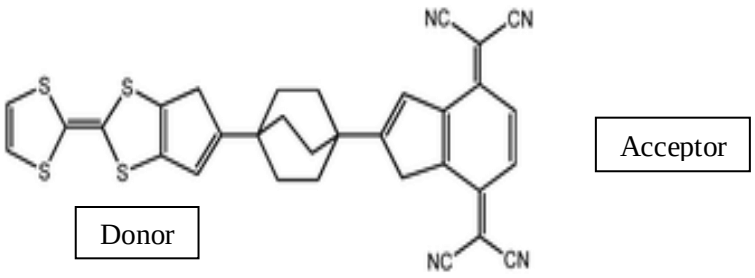


Fig 2.4.3 Molecular diode configuration

2.4 Summary

This chapter gives an overall idea how electron transportation is occurred as well as how it is related to molecular electronics; single molecule transistor also. It helps relating the other components such as molecular diode to gate terminal procedures to molecular transistor. It is now furthermore easier to understand the whole connection among the various topics discussed in the report in upcoming chapters.

Chapter 3

The "orthodox" theory of coulomb blockade is one the tools that has been successful in explaining and understanding the basic transport properties of semiconductor quantum dots. Using molecules as electronic segments is an effective new worldview in the science and innovation of nanometer-scale systems [12]. Examinations to date have analyzed a large number of particles leading in parallel [13, 14], or, sometimes, transport through single molecules [15, 16, 17, 18, 19, 20]. In the past two sections, we talked about single particle transistors produced using fullerene atoms, where electrons stream by jumping on and off the particle.

3.1 Overview to coulomb blockade theory

There are at this point numerous cases in nanophysics in which the electronic transport through a little question which is feebly coupled to metallic terminals has been investigated. Give us a chance to specify, for example, the instances of semiconductor quantum spots, carbon nanotubes or metallic nanoparticles. In every one of these frameworks, the vehicle in the feeble coupling administration is administered by single-electron burrowing forms that prompt wonders like the Coulomb blocked effect. Besides, if the coupling isn't so powerless, other fascinating many-body wonders, similar to the Kondo impact, can appear at indicate temperatures. We should find in this part these wonders additionally show up in single-atom intersections. These impacts have been comprehended in awesome detail in various devices with the assistance of an entryway terminal. This third terminal is

just capacitive coupled to the little question and it permits to tune its vitality level range and to investigate distinctive charge (or redox) states. The entryway cathode enables us thusly to control the present that courses through the framework with an outer field, especially like on account of field effect transistors in microelectronics. Because of this analogy and furthermore to the reality the transport is typically overwhelmed by single-electron forms, these pitifully coupled frameworks are known as single-electron transistors (SETs). In the most recent decade it has turned out to be conceivable to fuse a door cathode into single-atom gadgets. We should allude to these three-terminal sub-atomic gadgets as single-particle transistors (SMTs).

A definitive point of confinement would be where electrons bounce on to and off from a single atom between two contacts. In this section, we will say about transistors fusing a change metal complex planned with the goal that electron transport happens through all around characterized charge conditions of a single atom. Discuss the electronic transport through SMTs with special emphasis in the role of the Coulomb interaction in the molecules.

This part is composed in view of a formerly distributed paper [21]. Some portion of the content and figures are excerpted from the paper.

Coulomb blockade theory: Constant interaction model

A large portion of the outcomes got so far in single-atom transistors (SMTs), i.e. in weakly coupled three-terminal sub-atomic devices, have been broke down with the assistance of the "orthodox" hypothesis of Coulomb barricade [22], which has been extremely effective clarifying the fundamental transport properties of semiconductor quantum dots. Consequently, and before explaining a portion of the primary examinations reported to date, it is essential to talk about in certain detail this hypothesis, which is frequently alluded to as the steady connection demonstrate.

In the following subsections we exhibit an introductory explanation of the standard hypothesis of Coulomb blockade giving careful consideration to the significant administration for atomic devices.

3.2 Basic concepts of a single electron transistor with coulomb blockade theory

There are two suppositions of the constant interaction model that are not met when all is said in done in SMTs. Neither the charging energy nor the level ranges are required to be autonomous of the quantity of electrons in atom. In this sense, the standard hypothesis of Coulomb blockade may not be satisfactory for SMTs. The normal inquiry is currently how to sum up the standard hypothesis to manage atomic devices. It merits specifying that this inquiry has likewise developed in alternate settings like few-electron quantum dabs [23] and ultra-small metallic grains [24].

Some portion of the response to this inquiry is somewhat straightforward, in any event theoretically. Any hypothesis of Coulomb barricade in SMTs ought to incorporate a suitable depiction of the atomic many-body range as an element of the quantity of electrons in the particle. At the end of the day, we require as a beginning stage the ground state and energized conditions of the atoms for the unbiased species, as well as for the steady cations and anions.

On a fundamental level, this requires the utilization of ab-initio (post Hartree-Fock) quantum science strategies like, for example, the setup connection approach [25]. By and by, both model Hamiltonians and rough techniques like thickness useful theory have been utilized for this reason. Once the many-body range for various numbers of electrons is known, one needs to settle an ace condition to decide the control of the

diverse states lastly their commitment to the current. At this point many authors have implemented such a procedure at different levels of sophistication, and we just mention here a few works from which it should be easy to trace back the entire literature [26–37].

3.3 Summary

Another essential angle that a hypothesis of Coulomb blockade in SMTs should represent is the conceivable re-normalization of the sub-atomic levels because of the encompassing cathodes. The expansion energies discovered tentatively in SMTs are obviously considerably smaller than what is normal from the known ionization potential and the electron proclivity of the particles in gas stage. It has been recommended that this education of the expansion energies is caused by picture charges in the metallic terminals [38], offering ascend to a limitation of the charges close to the leads.

Chapter 4

In this chapter the most widely recognized techniques which have been created amid the most recent years for the manufacture of metallic atomic size contacts are mentioned. Both the reaching techniques and the physical properties of nuclear contacts found the reason for reaching single molecules. On the other hand, these strategies have been additionally refined for reaching molecules. These refinements are presently utilized for concentrate molecular contacts. The point of this section is to bring into the most essential standards and to analyze the procedures as to points of interest and disadvantages. In this manner, the choice in which section either strategy is portrayed is to some degree self-assertive. Complex varieties of the procedures exist and are for all time enhanced further.

4.1 Introduction to device fabrication

To perform the conductance measurement of an object, one needs no less than two terminals reaching the object- one for the source and another for the drain. For a tiny object, this requires a very simple experimental set. If they are bigger than 10 nm, the conductance can be measured. But for much smaller objects, conductance can be measured using electrodes that are fabricated by lithography methods or techniques.

The measurements of the conductance of a single molecule generally require a different experimental set up, because of their exceedingly small size. To measure the conductance of such tiny molecule, two electrodes (drain also source) would obliged

should bring a nm- size gap, so that they can “wire up” the atom. People have developed various new experiments for wiring up the single molecule.

4.2 Methods of fabrication

The contacting methods and the physical properties of the atomic contacts discovered that foundation for contacting single molecules. Varieties of the techniques exist and are permanently improved further. The aim here is to introduce the most important principles and to compare the strategies in regard to their preferences furthermore drawbacks. When dealing with tiny contacts, consideration need with be taken to decrease the influence of the estimation onto the contact itself.

4.2.1 Mechanically controllable break-junctions (MCBJ)

Many processes that enable the fabrication of atomic-size contacts and tunable tunnel contacts have been presented in days. The needle-anvil or wedge-wedge point contact technique pioneered by Yanson and co-workers in [39] included the first realizations. There was the squeezable tunnel junction method described by Moreland and Hansma [40]. There was also Moreland and Ekin [41]. These guys showed a different technique by using metal electrodes on two separate substrates which are then carefully adjusted with respect to each other. In order to form a contact with diameters of typically several nanometers, the needle-anvil technique was mainly used. Consisting of, hundreds or thousands of atoms in the narrowest cross section areas. Forming the development of the mechanically controllable break-junctions (MCBJ) which was proposed by C. Muller and coworkers in [42], these techniques established the beginning points, which nowadays play a vital role in the field of fabrication. Among them the most common ones are the so-called notched-wire [43] and thin-film MCBJs [44].

Components Needed For the Procedure:

(i) Metal wire,

(ii) The elastic substrate,

(iii) The insulating sacrificial layer,

(iv) The pushing rod,

(v) The counter supports and the dimensions used for calculating the reduction ratio.

Working Principle

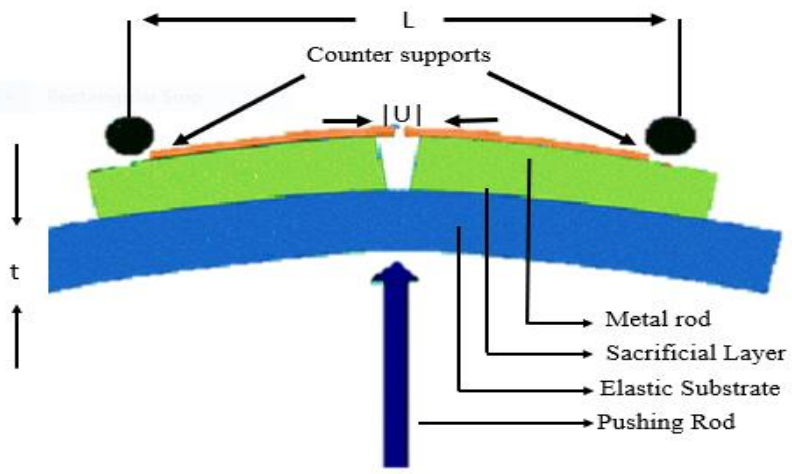


Fig 4.2.1 mechanically controllable break junction

The working principle shown in Fig. 4.2.1 is same for both types (notched-wire and thin-film MCBJs):

(1) Above a flexible substrate, a suspended metallic bridge is fixed on, which is mounted in a three-point bending mechanism which consists a pushing rod and two counter-supports.

(2) The position of the pushing rod relative to the counter supports. The counter support is controlled by either a motor or piezo drive or even with the combinations of both.

(3) The electrodes, above the substrate can be lengthened by increasing the bending of the substrate. The electrodes length can be reduced again by pulling back the pushing rod.

(4) For breaking a junction to the tunneling regime, significant displacements of the pushing rod and thus important bending of the substrate is required. So the most commonly used substrates are metals with a relatively high elastic limit. Example: spring steel or bronze. Before the junction can be fixed on it, the substrates are covered by an electrically isolating material such as polyimide.

4.2.2 Scanning Probe:

Theoretically, the most affordable method for contacting a single molecule with a fine tip is by depositing the molecule on a metallic substrate and by approaching the molecule with the tip until one or several atoms of the molecules is chemisorbed to the tip. But this method is suitable for handful amount of molecules and it isn't that much easy as it sounds. But even if we could do this successfully there lies the measurement issue because, in STM the electronic signal is convoluted with topographic information. Even the molecules can get destroyed by the presence of the tip. So, therefore a various STM techniques have been developed.

Fabrication steps:

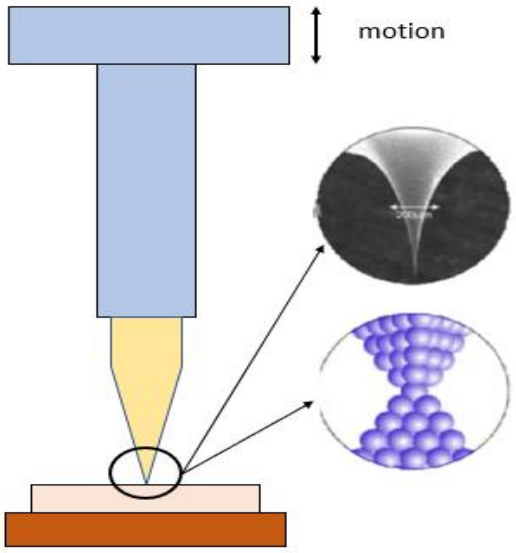


Fig 4.2.2

1) First needs careful preparation and characterization of the surface.
2) 2) Then a sub-monolayer of the molecules is deposited. By scanning the surface a suitable molecule is selected.
3) Depending on the physical question to study, an isolated molecule or a member of a larger aggregate can be chosen.
4) A fine metallic tip is held at distance from a counter electrode
5) The tip can also be indented into the surface and carefully withdrawn until an atomic size contact or short atomic wire forms.

Advanced Nano Fabrication

4.2.3 Electro-migration Technique

Another method for the fabricating of atomic-size contacts is controlled burning of a wire by electro-migration (see Fig 4.2.3). This technique has been optimized for the formation of nanometer sized gaps for trapping individual molecules or other Nano

objects which was discussed in [45, 46]. Before the wire finally fails and the current drops drastically, atomic size contacts are formed for a rather short time span [47–49].

Fabrication Steps

In order to fabricate atomic contacts a high threshold current is not important but the possibility for controlling speed, shape and size of the final structure.

(1) Defining the position and contact form

One of the most important preconditions is to define the position at which the electro migration starts, and the contact forms. For this purpose a short and thin metallic wire is fabricated by lithographic methods as described in the previous section. Typical dimensions are a length and width of 50 to 100 nm and a thickness of 10 to 20 nm. The thin wire is connected to wider and thicker electrodes which consequently have smaller resistivity.

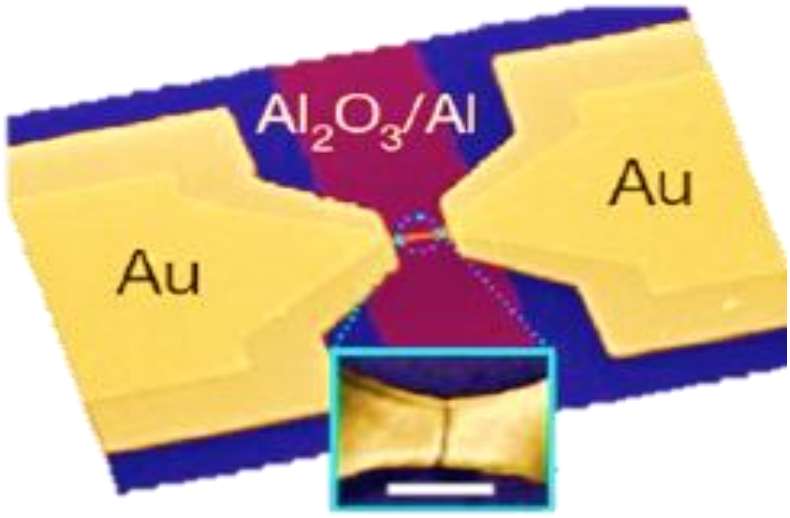


Fig 4.2.3 Electro migration technique

(2) Shadow Evaporation Through a Suspended Mask

i) First, thin layers of the metal are evaporated under the angles θ and −θ. The angle is chosen such that both layers slightly overlap underneath the suspended part of the mask.

ii) Then a thick layer of the electrode metal is deposited perpendicular to the substrate plane. The ideal structure would consist of a single-crystalline wire in the thin part of the wire, the boundaries of which are covered by the thick electrodes in order to avoid electro migration of possible contaminants from the grain boundaries.

4.2.4 Mask Evaporation

The self-alignment property of shadow masks is another method for fabricating small ensemble devices.

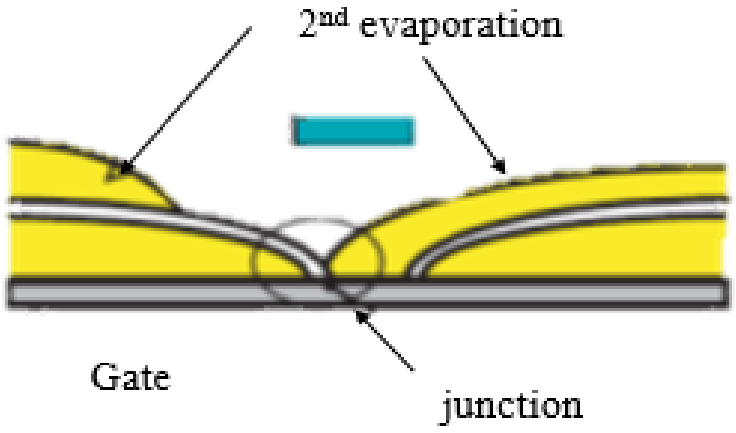


Fig: 4.2.4 mask evaporation technique

(1) Via e-beam lithography a suspended mask is produced with geometry of a wire that is interrupted by a small gap. A first metal layer is evaporated perpendicularly through this mask.

(2) The next step is the deposition of a SAM of the molecules. Alternatively molecules can be evaporated on top of the metal under the same angle.

(3) Subsequently a second metal layer is evaporated under an inclined angle such that the edge of the metal film covers the molecular layer.

Restrictions

(i) The resolution limits of the lithography used for the preparation of the mask restrict the contact size to roughly 50 nm in width. The overlay length is given by the evaporation angle and is usually chosen in the range of 20 to 50 nm. It has been shown that the smoothness of the first metal layer is mandatory for avoiding shortcuts between both electrodes.

(ii) A second problem of this method is the risk of destroying the SAM by the heat impact during the evaporation of the top electrode or of creating metal grains [50].

4.2.5 Gold Nano-Particle

A very elegant method for overcoming the size mismatch between the resolution of lithographic methods in use for the definition of the electrodes and the molecules has been described by T. Dadosh et al. in [51].

Fabrication Steps:

(1) The molecules to be contacted are functionalized at both ends with thiol anchoring groups, which have a high affinity to gold.

(2) By these thiol bonds the molecules are attached to the GNPs such that two of them are combined to form a dumbbell.

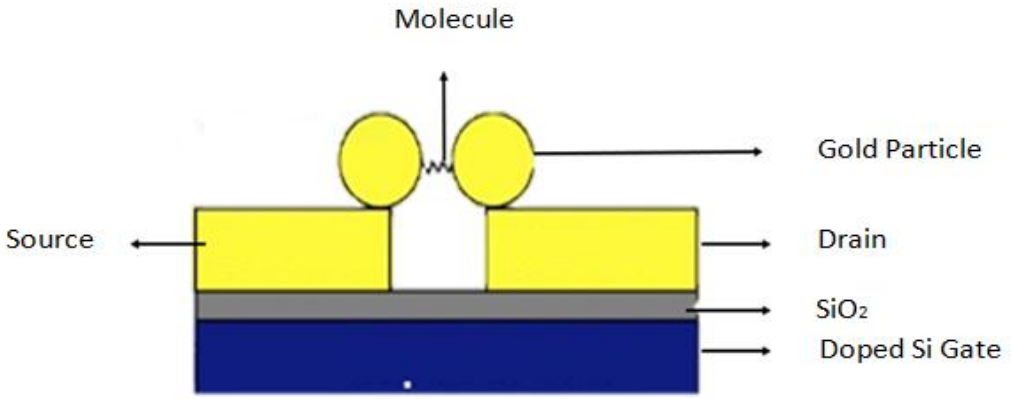


Fig: 4.2.5 Gold Nano-Particle

Those dumbbells now have a suitable size for bridging lithographically defined nanogaps and can be deposited onto them straightforwardly.

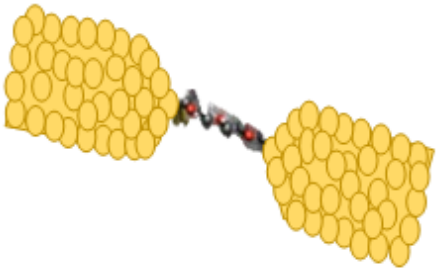
A further advantage of the method is that the statistical behavior of the molecules in contact with the GNPs can be studied by various non-contact methods such as optical spectroscopic measurements before deposition onto the electrodes (Fig.4.2.5).

4.2.6 Gold Nano-Rods:

Finally, it is possible to form networks of single-molecule junctions combining the robustness and statistical richness of ensemble studies with the fact that each junction

is formed by a single molecule or a very small number of molecules only which was talked about in [52, 53]. The fabrication scheme is shown in Fig. 4.2.6.

(1) Firstly gold nanoparticles (GNP) are covered with a spherical ligand shell. The thickness of the ligand shell corresponds to half the length of the molecules which shall be assembled between the GNPs later.



(2) Then a dense-packed, well-ordered, two-dimensional array, of these dressed GNPs is deposited onto a substrate which is subsequently patterned with metallic electrodes for performing the contacts to the measurement circuit.

Fig: 4.2.6 Gold nano rods

This kind of array contains approximately a million nanoparticles.

(3) The molecules forming the legend shell can be replaced with an exchange reaction by the molecules to be studied electrically.

The typical properties of an individual molecular junction can be at least partially deduced from the behavior of the network by using network analysis methods.

Chapter 5

Formulation and results as well as the related graph discussion is mentioned in this chapter. The description of each denotation is also mentioned here.

5.1 Formulation of a problem

Consider SET a transistor with the central grain which has a gap of 2Δ in the energy spectrum:

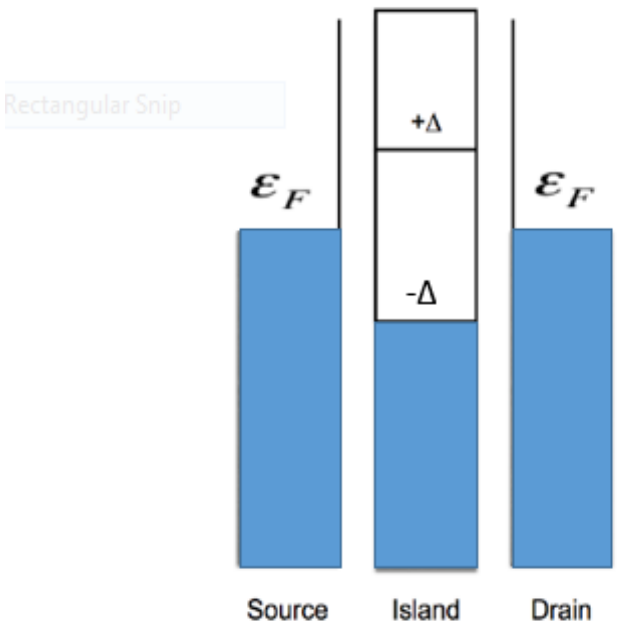


Fig 5.1.1 SET with energy gap on island

For this situation the main thing that adjustments in contrast with the conventional instance of metallic source, drain and island is the formulas for Γ. For proper occupation numbers for the electrons on the grain, we include the chemical potential. Chemical potential is given by the equation,

$$n_f(\varepsilon) = \frac{1}{\exp(\frac{\varepsilon - \mu(n)}{kT}) + 1}$$

And now if we set it according to the values of,

$$\mu(n) = \begin{matrix} \Delta \\ 0 \\ -\Delta \end{matrix} \quad for \quad \begin{matrix} n > 0 \\ n = 0 \\ n < 0 \end{matrix} \quad \text{where} \quad \Delta = \frac{e^2}{2C_\Sigma}$$

5.2 Formula derivation

We have to consider separately two cases for tunneling onto the grain (Γ1, Γ2) and out of the grain (Γ1, Γ2)

Now if we take that electron (hole) with energy ε before tunneling ends up with energy (ε + ΔK) and by integrating over energy values in the grain, we get the following derivation steps.

Given that,

$$\vec{\Gamma} = \int_{-\infty}^{\infty} n_{Fs}(\varepsilon)(1-n_{Fi}(\varepsilon+\Delta\vec{K}))d\varepsilon$$

Changing the variables, we get

$$\varepsilon' = \varepsilon + \Delta\vec{K} \;\; \varepsilon = \varepsilon' - \Delta\vec{K}$$

We know, $I = \frac{2e}{\hbar}\frac{\Gamma_{i;L}\Gamma_{i;R}}{\Gamma_{i;L}+\Gamma_{i;R}}$ and

$$\Gamma = \frac{G}{e^2}\frac{kT}{(1-e^{(\mu-\Delta K)/kT})}\ln\left[e^{\frac{\Delta K-\mu}{kT}}\left(\frac{e^{\frac{\mu}{kT}}+e^{\frac{-\Delta}{kT}}}{e^{\frac{\mu}{kT}}+e^{\frac{\Delta}{kT}}}\right)\left(\frac{e^{\frac{\Delta K}{kT}}+e^{\frac{\Delta}{kT}}}{e^{\frac{\Delta K}{kT}}+e^{\frac{-\Delta}{kT}}}\right)\right]$$

$$I(V) = \frac{2e}{h}\int_{-\infty}^{\infty} dE\, T(E,V)\,[f(E-eV/2) - f(E+eV/2)]$$

So, we get

$$\vec{\Gamma} = \int_{-\infty}^{-\Delta} n_{Fs}(\varepsilon-\Delta\vec{K})(1-n_{Fi}(\varepsilon))d\varepsilon + \int_{\Delta}^{\infty}(...)d\varepsilon$$

Similarly,

$$\overleftarrow{\Gamma} = \int_{-\infty}^{-\Delta} n_{Fi}(\varepsilon)(1-n_{Fs}(\varepsilon+\Delta\overleftarrow{K}))d\varepsilon + \int_{\Delta}^{\infty}(...)d\varepsilon$$

Solving the integrals, we get

$$\Gamma_{in} = \frac{kT}{1-\exp(\frac{\mu-\Delta\vec{K}}{kT})}\ln\left(\frac{e^{-\Delta}+e^{\mu}}{e^{-\Delta}+e^{\Delta\vec{K}}}\frac{1}{\exp(\frac{\mu-\Delta\vec{K}}{kT})}\frac{e^{\Delta}+e^{\Delta\vec{K}}}{e^{\Delta}+e^{\mu}}\right)$$

$$\Gamma_{out} = \frac{kT}{1-\exp(-\frac{\mu+\Delta\vec{K}}{kT})}\ln\left(\exp(\frac{\mu+\Delta\vec{K}}{kT})\frac{e^{-\Delta}+e^{-\Delta\vec{K}}}{e^{-\Delta}+e^{\mu}}\frac{e^{\Delta}+e^{\mu}}{e^{\Delta}+e^{-\Delta\vec{K}}}\right)$$

Results and discussion

Figure below demonstrates the 4 plots for understanding the coulomb blockade impact. The 1st chart is the current versus Voltage diagram. The straight line in the center can be viewed as the coulomb blockade impact. So also, in the second plot for conductance at a particular Vb; the dip in the diagram is the impact. The third chart is that of current versus Vb versus Vg, and the last diagram is the conductance diagram, that particularly demonstrates the Coulomb Blockade impact in blue.

Default parameters:

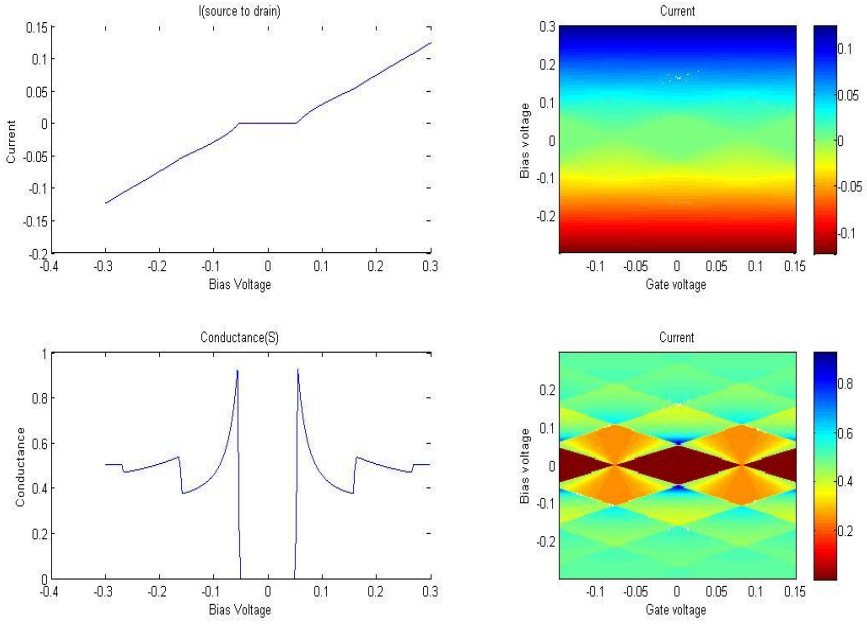
$C_1 = C_2 = C_g = 1x10^{-18}$ F;

T = 20 K;

n=(-10:10);

$G_1 = G_2 = 1$;

$\Delta = \frac{e^2}{2*\sum C} = 2.52$ meV;



Default parameters:

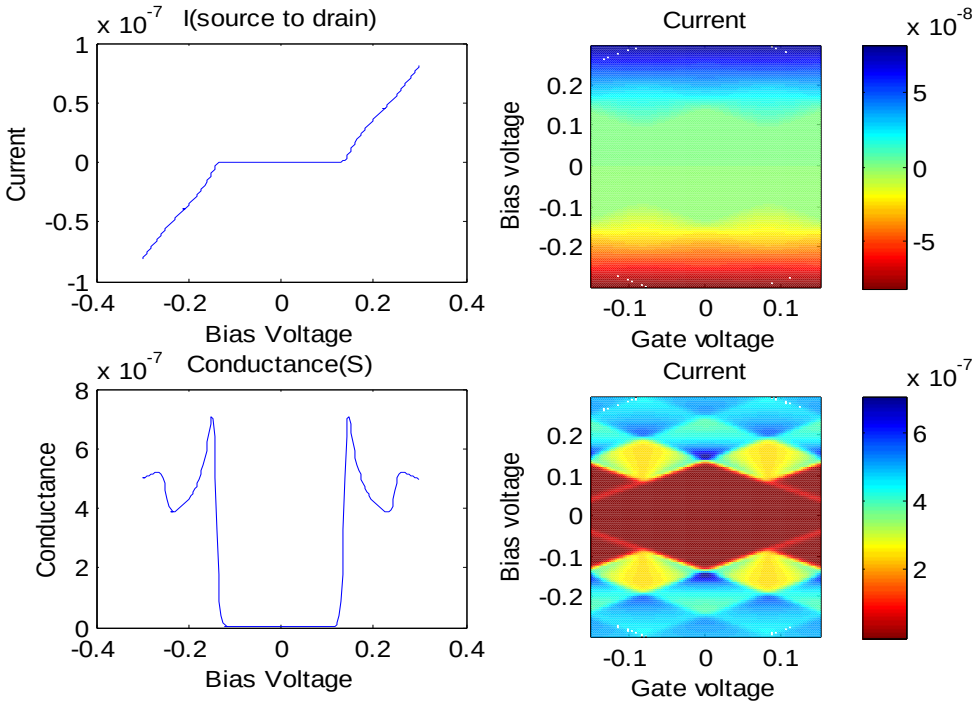
$C_1 = C_2 = C_g = 1x10^{-18}$ F;

T = 20 K;

n=(-10:10);

$G_1 = G_2 = 1 \text{ X } 10^{-6}$;

$\Delta = \frac{e^2}{2*\sum C} = 2.52$ meV;


x 10^-7 I(source to drain)
Current
Bias Voltage
x 10^-7 Conductance(S)
Conductance
Bias Voltage
Current
x 10^-8
Bias voltage
Gate voltage
Current
x 10^-7
Bias voltage
Gate voltage

Conclusion

In this thesis we discussed the fabrication and the measurements of single molecule transistors where electrons burrow one by one through the particle. We found that electrical conductance changes relying upon how tunneling electrons communicate with different quantum excitations of the atom. One can apply the aftereffects of this proposition to explore the electronic movement in single atoms and furthermore to outline new particles that have valuable properties for novel electronic devices.

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