CHAPTER 7

SUMMARY AND OUTLOOK

7.1 OUR MODELING IN MOLECULAR DEVICE

We have adopted semi-empirical formalism for describing nanoscale conduction in various molecular systems. The molecular device is described through an appropriate Hamiltonian. Coupling with the contacts is described through self energy matrices once again using an appropriate Hamiltonian described of the contact atoms, and taking into account the surface bonding geometry as well as the contact crystalline arrangement. Finally a set of NEGF transport equations are utilized to describe nonequilibrium transport under bias through the conduction level of the device.

We focused our attention on qualitative description of transport through molecule based junctions. Calculations of transport characteristics were performed using Extended Hückel Theory (EHT) and simplified charging model in the computational scheme based on Non Equilibrium Green Function (NEGF) formalism.

In this work, we modeled our molecular junctions using single molecule like dimethanethiol, biphenyldithiol, alkanedithiol, amino alkanethiol, pyrole, furne, thiophene, borazine, BCN unit structure and Tour wire, which are sandwiched between two clusters of gold atoms. The results of our modeling yields physical insight into conduction and these theoretical results will help to design future electronic devices.
7.2 VALIDATION OF RESULTS

Based on the present theoretical investigation using semi-empirical formalism for various molecular junctions, the following conclusions are drawn:

The changes in the charging energy cause dramatic effect on the transport properties in the conductance spectra. With the increase of U parameter, the charging reduces the height of conductance peaks, broadens the peak in conductance spectra and smoothening the I-V characteristics. The effect of torsion angle on the transport characteristics shows that BDMT and BPDT molecule can be used as a switch. In these systems, the electronic switching action which control the conservation between state 0 (open state) and state 1 (closed state) can be achieved due to the rotation of the molecule with a torsion angle with respective to the gold leads.

The chain length effect on fully saturated molecules like alkanedithiol molecules and the conjugated molecular family of heterocyclic molecules such as pyrrole, furan and thiophene wire shows that increasing the chain length of the these molecules increasing the tunneling decay rate, which leads the decrease in conductance. Also the transport through a fully conjugated bridge is greater than through a saturated bridge. These results are excellent agreement with “rules of thumb” for electron transport in molecular systems.

The effect of terminal groups and the coupling to the contact offer the possibility of modifying their transport behavior in a controlled way and can improve/add some functionality for the design of molecular electronic devices. For heterocyclic molecules, in the weak coupling limit current shows stair case like structure, while it gets a continuous variation in the strong coupling limit. Negative differential resistance behavior was observed for borazine-CN molecular junction, which is of agreement with the experimental observation.

For Tour wire systems, by varying the temperature negative differential resistance (NDR) behavior was obtained at 100K, which is comparable with the
experimental results. The conductance of Tour wire systems is tuned by the lead induced thermal broadening or configurational thermal broadening.

The method described and used here can easily be applied to different molecular devices. As this model is based on semi-empirical method it is computationally inexpensive and flexible, yet at the same time it is able to capture salient qualitative features as well as several relevant quantitative details of transport. The method used here provides not only the physical interpretation of experiments, but also information about the formulation of charge transport in single - molecular junction.

The present investigation emphasized that, designing a molecular device is strongly influenced by the molecular geometry, molecule - to - electrode interface structure, molecular chain length as well as molecular coupling strength.

7.3 FUTURE DIRECTIONS

Although major advances have been made, the current state is quiet mixed because of many computational assumptions. Density functional Theory (DFT) treatments can avoid this by self consistent analysis.

Three terminal devices and providing one specific molecule will different functional parts of performing different tasks can be simulated. Though single molecular transistor has been studied, investigation is required to study the interaction of tunneling electrons with various quantum excitations of the molecule to design novel electronic devices.

However unimolecular rectification has been fully confirmed, exploration is required to see if rectifiers and strands of conducting polymers be grafted together to form a molecular transistor with power gain.

A new era of the molecular level engineering instead of the band engineering will come soon.