

Several electronic applications of organic materials have been discussed in this work as a single molecule device. However, a more complex system of the single molecular devices needs to be designed for commercial purposes. This chapter will summarize our contribution in understanding and advancement of single molecule device design along with concluding remarks and future of the technology.

### 7.1 Summary

The silicon technology failed to maintain Moore's law of miniaturization mainly due to quantum mechanical effects and limited cutting-edge technologies. Therefore, several other technologies arise as alternatives. Organic materials based single molecular device design emerged as a strong contending technology due to several advantages like: low power consumption, flexibility, scaling, cost effectiveness and ease of utilization of organic materials. In this thesis several aspects of single molecule organic device design were explored while keeping in mind the potential usability of the subject matter in futuristic electronic market. The technology is in early stage of development and therefore several goals have to be achieved before mass production and commercial utilization of the end product. Keeping that in mind some experiments were executed and these inferences were gleaned;

- I. The very first step for designing a single molecule device is selection of the molecule itself. In this case we opt for organic materials because of their several advantages mentioned above. However, there are plenty of organic materials that can be examined for this purpose.
- II. The redox active organic materials have proven their usability in several electronic applications. Most of these materials are equipped with various functional groups which enhances electronic properties of base molecule.
- III. DFT calculations are also very helpful to examine small sized molecules. This will drastically reduce amount of resources put on experimenting with these molecules. However, same is not the case with large sized molecules or polymers. It turns out to be very difficult for DFT simulators to converge large space of big molecule configuration.
- IV. Several parameters need to be identified before putting a molecular device configuration to testing. First and foremost, of these parameters is the configuration of molecule which must be energy relaxed. User defined coordinates values play huge role in the convergence of device space. Later on, interatomic force can reach to local minima value with FIRE, Quasi-Newton or LBFGS methods.
- V. DFT calculations are a complex set of equations which involve trade-off between computation time and accuracy. Therefore, optimum value of certain parameters like mesh cut-off energy and k-point sampling value must be determined to maintain desired accuracy of the results. Some other parameters include selection of boundary conditions, choice of basis sets, electron temperature and above all type of exchange correlation.

- VI. After selection of desired parameters, certain analysis needs to be performed first on molecule and later on entire device configuration. These analysis include molecular energy spectrum and total energy spectrum for molecule to calculate HOMO-LUMO energy states and electron affinity/ionization energy respectively. While device-based analysis includes calculation of density of states, molecular projected self-consistent Hamiltonian and transmission spectrum.
- VII. Finally, current-voltage characterization has been performed within voltage range from -3V to 3V. Bidirectional multiple negative differential resistance (BM-NDR) was observed on 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ). Based on the IV data generated after DFT calculations several finite bias analysis have been evaluated on peak and valley voltages. As a result, the BM-NDR phenomenon has been concluded to be caused due to double reduction and contact resistance between electrodes and molecule.
- VIII. Now we came to know the possible electronic application of DDQ molecule therefore further efforts were made for the experimental realization of DDQ based single molecule device. For that purpose, Scanning Tunneling Microscopy (STM) system was used. Mica/Au has been chosen to serve as substrate as well as bottom contact of the device and Pt-Ir tip as top contact as well as for topographic imaging of the deposited molecules. For deposition of DDQ molecule in-situ e-beam evaporator was used and to remove residual or loosely bounded molecules on the substrate in-situ sputtering system and PBN coated heater were used.
- IX. During topographic imaging of the DDQ deposited substrate several phenomena were observed like; self-assembly of DDQ molecules, transfer of surface tension from substrate to self-assembly of DDQ molecule in the form of herringbone structure, BM-NDR behavior of single DDQ molecule and unconventional molecular counter outcome due to supra-molecular structure of the molecules.
- X. Another experimental analysis has been performed on newly synthesized polydentate Schiff's base ligand. The single molecule analysis reveals rectification and memory switching nature of the ligand molecule. Topographic imaging of ligand molecule drop-casted on mica/au surface divulge the formation of branched monolayer structure of ligand molecules

## 7.2 Concluding Remarks

After detailed theoretical and experimental analysis and several observations this can be concluded from this thesis work that organic molecules have immense potential to be used as single molecular device. Though the theoretical analysis is a trade-off between computation time and accuracy therefore a lot can further be investigated by using more accurate functionals but with experimental verification of theoretical prediction one can rest assure about the electronic properties of the DDQ molecule. Moreover, with experimental observations we came to know about the strange property of self-assembled monolayer of DDQ molecules which make it useful as an unconventional asynchronous counter. During this experimentation with proper utilization of several parameters of e-beam lithography, RF sputtering and PBN heater we were able to reduce the thickness of the active material to monolayer scale. Same scale has been achieved on a comparatively large sized non-planer ligand molecule. The ligand molecule was synthesized by our collaborators and we were successfully able to characterized their electrical properties at molecular scale using STM system. The IV results gained with gold substrate and tungsten tip on ligand molecule suggest formation and breakdown of dative bonds which ultimately is responsible for the rectification and memory switching behavior of the ligand molecule. All of these results and observations indicates towards the bright future of organic molecules as single molecule device for the development of highly scaled electronics integrated circuits.

### 7.3 Future Scope

The main aim to carry out this research was revolving around the identification and verification of potential usability of organic materials in the development of single molecule device design. Certainly, two of the organic materials have been tested in this thesis as potential applicant of single molecule device. Yet many more organic materials need to be identified as well as tested for the same purpose. Apart from that a lot can be improved in several areas to further enhance the quality of the testing. These areas include:

- I. More accurate exchange functionals like GGA and Meta-GGA can provide far accurate results as compared to LDA. Though the improved accuracy will come with improved computation time as well.
- II. Utilization of other in-situ fabrication and device preparation units like molecular beam epitaxy, atomic layer deposition, and e-beam lithography within STM system will certainly enhance the quality of device design and material deposition.
- III. Though most practically used electronics devices have application on room temperature but from physics point of view we learn more about the properties of a material by rejecting thermal noise due to room temperature. Therefore, effect of temperature dependency of the organic materials on their electronic properties must be very helpful.

