

Contents

	<i>Page</i>
<i>Abstract</i>	vii
<i>Acknowledgements</i>	ix
<i>Contents</i>	xi
<i>List of Figures</i>	xv
<i>List of Tables</i>	xix
<i>List of Symbols</i>	xxi
<i>List of Abbreviations</i>	xxiii
Chapter 1: INTRODUCTION	
1.1 Motivation	1
1.2 Single Molecule Organic Electronics (SMOE)	2
1.2.1 Applications	3
1.2.2 Types of organic molecules	3
1.2.3 Electronic charge transportation in molecular devices	4
1.2.4 Effect of conjugation on charge transport mechanism	6
1.2.5 Device Structure	7
1.2.6 Quantum effects in molecular devices	7
1.3 Advancement towards organic molecular devices	9
1.4 Research focus and thesis organization	12
Chapter 2: Experimental Techniques and Instrumentation	
2.1 Theory of quantum tunneling	13
2.2 Design of STM System	14
2.3 Components in STM System for in-situ growth	15
2.3.1 e-beam evaporator	16
2.3.2 Crystal Monitor	17
2.3.3 Thermal/Direct Current Heating	18
2.3.4 RF Sputtering system	18
2.3.5 Cryogenic Chamber	19
2.3.6 Tip-preparation tool	20
2.3.7 Molecular beam pulsed valve source	21
2.3.8 Ultra High Vacuum (UHV) Condition	22
2.4 Device Characterization	23
2.4.1 Data Acquisition	24
2.4.2 Data Analysis	24
Chapter 3: Theoretical Background of Molecular Devices	
3.1 Introduction to Virtual NanoLab (VNL)	26
3.1.1 Builder	26
3.1.2 Scripter	27
3.1.3 Editor	28
3.1.4 Job Manager	28
3.1.5 Viewer and analyzer	29
3.2 Simulation methodologies	30
3.2.1 First principle method	30
3.2.2 Density Functional Theory (DFT)	30
3.2.3 Exchange Correlation Functionals	31
3.2.4 Non-Equilibrium Green's Function (NEGF)	32
3.3 Work Flow of Nano-Language Scripting	32
3.3.1 Molecular device configuration	33
3.3.2 Analysis	33
3.3.3 I-V characterization	34
3.3.4 Post-characterization analysis	34

Chapter 4:	Bidirectional Multiple Negative Differential Resistance (BM-NDR): A Theoretical Study of Molecular Device	
4.1	Introduction	35
4.2	Experimental	36
	4.2.1 Computational methodology	36
	4.2.2 STM Study	38
4.3	Results and Discussions	38
	4.3.1 Theoretical I-V study and zero bias transmission	38
	4.3.2 Experimental I-V characterization	40
	4.3.3 Transmission spectra and LDDOS	41
	4.3.4 Molecular Projected Self Consistent Hamiltonian (MPSH) orbitals study	42
	4.3.5 Characteristics of singly and doubly reduced DDQ molecule	43
4.4	Analysis	46
4.5	Conclusions	47
Chapter 5:	Voltage Induced Molecular Motors Constitute the Smallest Self-Assembled Molecular Electronic Counter: An experimental Study of Molecular Device	
5.1	Introduction	49
5.2	Experimental	50
	5.2.1 Deposition of Au on mica surface	50
	5.2.2 Deposition of DDQ on Au/mica surface	50
5.3	Computational Methodology	51
5.4	Results and Discussions	52
5.5	Analysis	61
5.6	Conclusions	62
Chapter 6:	STM study of Bias-Triggered molecular rectification and switching in Metal-ligand complex	
6.1	Introduction	63
6.2	Experimental	64
	6.2.1 Synthesis of Ligand	64
	6.2.2 Deposition of Gold on mica substrate	65
	6.2.3 Deposition of ligand on Au/mica substrate	65
6.3	Results and Discussions	65
	6.3.1 Physical properties of ligand	65
	6.3.2 Electrical Properties of Ligand	67
6.4	Conclusions	69
Chapter 7:	Conclusion	
7.1	Summary	71
7.2	Concluding Remarks	72
7.3	Future Scope	73
Annexure A:	Nano-Language Scripting	
A.1	Parameter optimization python script	75
	A.1.1 Python script of a molecular device configuration	75
	A.1.2 Python script for geometry optimization of molecular device	79
	A.1.3 Python script for the calculation of mesh cut-off energy for the atomic configuration	80
	A.1.4 Python script to determine k-point sampling values at different energy values	81
A.2	Molecule/Device Analysis Python Script	82
	A.2.1 Python script for electrostatic difference potential, total energy and molecular energy spectrum analysis	82
	A.2.2 Python script for eigen state analysis near fermi energy level as calculated from the log file of molecular energy spectrum analysis	83
	A.2.3 Python script for zero biased transmission spectrum analysis of molecular device configuration	84
	A.2.4 Python script for calculation of device density of states	86

A.2.5 Python script for calculation molecular projected self-consistent Hamiltonian (MPSH)	87
A.2.6 Python script for the calculation of transmission eigen values near fermi energy level as obtained from the analysis results of MPSH and their corresponding transmission eigen states	89
A.2.7 Python script for the calculation of the local device density of states analysis	93
A.3 Parameter optimization python script	95
A.3.1 Python script for I-V characterization of the molecular device configuration	95
Annexure B: Nano-Language Scripting	
A.1 Parameter optimization python script	75
References	99

