ABSTRACT

A computer system is made up of computing devices typically electronic logic gates and circuits. These devices basically facilitate the various computing operation inside a computer. In this regard the research work carried out and reported in this thesis based on the design and operational aspects molecular computing devices. These computing devices are basically electronic devices made from organic molecules or biomolecules.

This thesis is concerned with the problem of devising various means and methodologies as to design molecular devices in order to develop a molecular computer. The objective is whether it is possible to develop a single big molecular (or structural) formula which would act as a super computer.

In order to achieve these objectives, efforts have been made to design basic molecular building blocks, especially logic gates like AND, OR, NAND, NOT, NOR, XOR and XNOR. It has further extended to design molecular combinational circuits and their derivatives like Half adder, Full Adder, Multiplexer and Demultiplexer. The molecular sequential circuits like Flip-Flops, Counters & Registers have been designed to make them suitable as computing devices for molecular computer.

In order to develop a systemic approach for designing molecular electronic devices, a novel theory of Molecular Electronics System Model and Molecular Programming Pseudocode has been proposed here in this thesis in the framework of computational chemistry. The molecular orbital structure analysis has been carried out with help of Hartree-Fock method to determine the energy levels of orbitals. A simulation approach has been attempted using Molecular Monte Carlo Algorithm for arbitrary choice of molecule. The quantum conductance properties of the molecule have verified through Landeaur formula. The Volatge~Current characteristics have been formalized using fundamental theories of Density Functional Theory and Green’s function.

A little analysis has been done on DNA based computing devices like YES, NOT, AND, NAND, OR, NOR, XOR and Half-adder using deoxyribosome. At last a comparative study between silicon based computing devices, organic based computing devices and DNA based computing devices has done with respect to various performance factors responsible for designing a computer.