" QUANTUM TRANSPORT PHENOMENA IN MODULATED SEMICONDUCTOR HETEROSTRUCTURE BY USING DENSITY FUNCTIONAL THEORY "

INTRODUCTION:

The research aims to investigate " Quantum Transport phenomena in modulated semiconductor heterostructure and also to calculate electronic structure using Density Functional Theory " are of great importance for developing next generation electronic and quantum devices. The study of modulated semiconductor heterostructure such as Superlattices , Quantum well, Quantum dots that offers into coherent transport and quantum interference effectiveness.

OBJECTIVES:

To develop analytical and numerical models to study quantum transport in modulated semiconductor heterostructure and to calculate electronic structure .

MODULATED SEMICONDUCTOR HETEROSTRUCTURE:

These are the heterostructure where the potential or composition varies periodically or aperiodically. It can be achieved through Doping profiles, layer thickness variation,external electric and magnetic fields, lattice mismatch .

DENSITY FUNCTIONAL THEORY:

DFT is a quantum mechanical method used to calculate the electronic structure of molecules. It simplifies the many body problem of electrons by using the electron density rather than wave functions. For transport,to calculate electronic states and potential profiles to using density functional theory . To combine with non equilibrium Green's function formalism for transport calculations.

LITERATURE REVIEW:

Semiconductor heterostructure like (GaAs/AIGaAs and InGaAs/Ip) or(InP/ Gasb/ Inp) in the presence of laser propagation have been studied for the quantum transport characteristics. Past studies have demonstrated mini band formation of semiconductor heterostructure and the role of quantum interference in one dimension and two dimensions. More recent studies involve topological insulators and quantum hall systems , highlighting the rich transport phenomena in modulated heterostructure. And the model such as tight binding approach and Non equilibrium Green's function (NEGF) methods widely used to analyse electron dynamics. The combined effects of modulation and electron coherence in heterostructure remain best for exploration.

METHODOLOGY:

- We can find theoretically relative strength of electric field due to laser by Schrödinger equation and effective mass approximation for quantum well or superlattice structure.
- Transfer Matrix Method by MATHCAD for transmission coefficient calculations.
- To combine DFT, with non- equilibrium Green's function can describe quantum transport (ie) current flow under bias, non equilibrium Green's conditions.
- Use code like Quantum EXPRESSO for DFT calculations.
- DFT WITH NEGF is a powerful approach for investigating the quantum transport characteristics behaviour in modulated semiconductor heterostructure with some limitations.