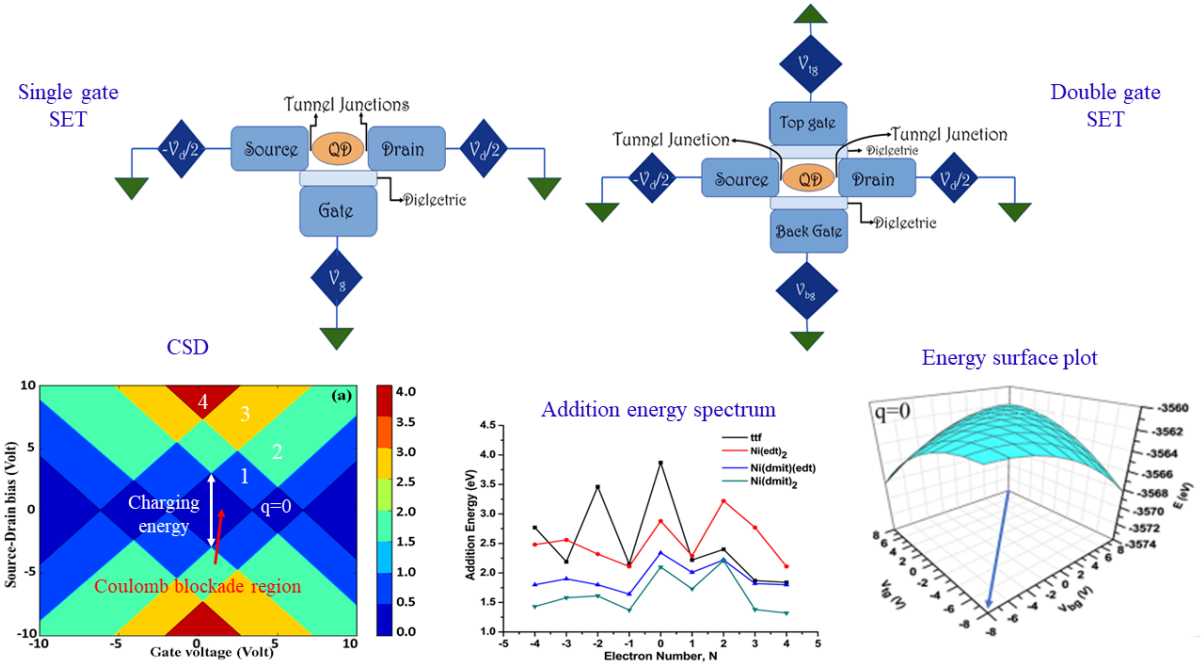
Name of Ph.D. student:	Anu
Name of Supervisor:	Prof. Mohd. Shahid Khan
Name of Co-supervisor:	Prof. Anurag Srivastava
Department:	Physics
Title of the Thesis:	Investigations of Metal-Organic Complexes for Electronic and Optoelectronic Applications

Abstract

The thesis mainly presents the investigations for metal organic complexes for electronic and optoelectronic applications using density functional theory (DFT) formalism, modelling them as islands in Single Electron Transistor (SET) devices, calculating their nonlinear optical properties, and performing principal component analysis (PCA) for all the studied molecules.



To model SETs, the Metal organic complexes owing to their enormous potential application in optoelectronic devices, have been used and successfully investigated for the next generation technology. The selected molecules and derivatives based on thiophene have been used for this purpose. All the studied molecules have been optimised to their ground state structure using DFT with B3LYP method with 6-311G and LanL2DZ basis sets, bringing the atomic level understandings of the structures of complexes, before modelling them as islands in SETs.

Studying the SETs forms a major part of the thesis, for which the metal organic complexes of thiophene and dibenzothiophene as islands in SET are studied for the transport properties, Effects of dielectric material and electrode material represented that metal organic complexes (Cr-complex of thiol-ended thiophene, Cr-complex and W-complex of thiol-ended dibenzothiophene) gives improved conductance than their base molecules. Also, Ni-dithiolene derivatives are modelled as SETs and analysed for their charge stability diagram and addition energy spectrum to conclude that $Ni(dmit)_2$ molecule has better conductive nature than other studied Ni-dithiolene derivatives.

Another work performed is Gate morphology trying to understand the effects of additional gate to the SET configuration, for which the surface plots of energies have been studied for Vanadium tris(dithiolene) molecule and is found that energy values are lower for double-gated SET, and hence making it more conductive than single gated SET. And the sensitive nature of SET energy towards small gate voltages change proposes SET as a sensitive charge detector.

Further, the metal organic complexes of dibenzothiophene have also been studied for the optoelectronic properties. And a Principal Component Analysis (PCA) of all the studied molecules has been performed to derive a conclusion on the effects of different parameters on non-linear optical (NLO) properties.

Keywords: DFT, Metal organic complexes, SET, Sensor, Optoelectronic properties, PCA.