

## **Annexure A**

### **Days    Contents (QP-Quantum Physics, SSP- Solids State Physics)**

- Day-1    Molecular Modeling and Scope of Density Functional Theory(DFT).
- Day-2    Pre-Processing Tools for DFT Studies. Installation of tools
- Day-3    Introduction of Linux and Some Basic Commands : Hands on Training
- Day-4    Comparative analysis of various DFT-Tools introduction of SIESTA tool.
- Day-5    How to read a research article and make research plan for project/dissertation ?
- Day-6    QP-I : Wave Particle Duality, Quantum States and Wave Function.
- Day-7    QP-II:Schrodinger Equations : Time Dependent and Time Independent.
- Day-8    SIESTA introduction and Installation-Series and Parallel : Hands on Training
- Day-9    Discussion,Problems and Solutions.
- Day-10    QP-III : Application Schrodinger Equation (Particle in a box).
- Day-11    QP-IV : Variational Principle and Hamiltonian. Two body problem
- Day-12    SSP-I : Basics of Solis State Physics in Context of DFT. Various Solid State Devices.
- Day-13    How to Create SIESTA input fdf file ? : Hands on Training
- Day-14    Discussion,Problems and Solutions.
- Day-15    SSP-II : Periodic Structure, Supercell and Lattice Parameters
- Day-16    SSP-III: Crystal Structures, : Lattice, Lattice Vector, Basis, Unit Cell, Bravais Lattice.
- Day-17    SSP-IV: Miller Indices for Crystallographic Points and Directions.
- Day-18    How to use Xmgrace plotting tool? :Hands on Training
- Day-19    Discussion,Problems and Solutions.
- Day-20    SSP-V: Bonding in solids : Cohesive and Binding Energy, Defects, Band Theory of solids

- Day-21 DFT-I : Born–Oppenheimer approximation Hartee-Approximation, Hartree-Fock Approximation.
- Day-22 DFT-II: Thomas-Fermi Model, Hohenberg-Kohn theorems, Kohn-Sham equation.
- Day-23 How to use GDIS and VESTA tools ? :Hands on Taining
- Day-24 Discussion and Problems and Solutions.
- Day-25 DFT-III : Basis Sets and Pseudopotential, Exachange correlation Functions and self consistency.
- Day-26 DFT-IV : various optoelectronic devices fundamentals and characteristics
- Day-27 Structural/geometry optimization using SIESTA : Hands on Training
- Day-28 DOS/PDOS analysis-plotting and interpretaton of result : Hands on Training
- Day-29 Bands analysis-plotting and interpretaton of result : hands on Taining
- Day-30 Optical Properties analysis : plotting and interpretaton of result : Hands on Training