CHM621: Advances in X-ray crystallography and its applications [Cr: 4, Lc:3, Tt:1/Lb:1]

Course Outline: This course covers advanced topics in X-ray crystallography emphasizing the modern methods of structure determination and refinement, handling of X-ay diffraction data for charge density analysis, basics of experimental and theoretical charge density analysis, using the packages for charge density analysis (theoretical and experimental). The aspects of crystal growth, polymorphism, intermolecular interactions, multi-component crystals, in situ crystallization, crystal engineering, synthon approach, MOF and COF etc. will be covered under Crystal Engineering.

- **Basics of X-ray crystallography: Crystallographic symmetry, point groups and space groups, Bragg's law for X-day diffraction, data collection, data processing, structure solution and refinement, fixing of H atom and structure completion.**
- **Scope of structure analysis from routine data and need for high resolution X-ray.**
- **Introduction to experimental charge density study, breakdown of independent atom model, improved scattering model, Kappa formalism, multipole refinement methods, residual density, deformation density.**
- **Topological analysis of charge density data.**
- **Data collection and data processing strategies for charge density analysis through hands-on using a diffractometer.**
- **Introduction to XD and MoPro packages for experimental charge density analysis.**
- **Introduction to Crystal14 theoretical charge density analysis.**
- **Introduction to Crystal Engineering, organic solid state chemistry, modern aspects of crystal engineering.**
- **Intermolecular interactions and their applications in designing desired crystalline supramolecular architecture.**
- **Polymorphism, origin and thermodynamics of polymorphism, properties and applications of polymorphs.**
- **Multi-component crystals, pharmaceutical and non-pharmaceutical co-crystals, their importance, and applications.**
- **Metal-organic framework and covalent-organic framework materials and their applications.**
- **Quasicrystals.**
- **Introduction to macromolecular crystallography: Basics, choice of radiation, MIR, SAD and MAD phasing in protein crystallography, structure refinement.**

Recommended Reading:

- **G. H. Stout and L. H. Jensen, "X-ray Structure Determination A Practical Guide", 2nd Ed, Wiley Interscience.**
- **C. Hammond, "The Basics of Crystallography and Diffraction", IUCr Texts on Crystallography 12, 3rd Ed, Oxford Science Publications.**
- **P. Müller *et. al.*, Ed. By P. Müller, "Crystal Structure Refinement A Crystallographer's Guide to SHELXL", IUCr Texts on Crystallography, Oxford Science Publications.**
- **P. Coppens, "X-ray Charge Densities and Chemical Bonding", IUCr Texts on Crystallography 4, Oxford Science Publications.**
- **G. R. Desiraju, "Crystal Engineering A Textbook", World Scientific.**
- **J. Bernstein, "Polymorphism in Molecular Crystals", IUCr Monograph on Crystallography 14, Oxford Science Publications.**
- **Jan Drenth, "Principles of Protein X-Ray Crystallography", Springer; 3rd ed. 2007.**