Research on various types of materials using experimentally measured physical and structural data employing different computational techniques is going on as follows.

**DMS (Dilute Magnetic Semiconductor) materials**

One of the ongoing research work aims at studying the Diluted Magnetic Semiconductors (DMS) in terms of the structure, physical and electronic properties. The characterization techniques involve X-ray diffraction, magnetic characterization and other physical characterization like conductivity measurements etc.

The semiconductor materials doped with small amount of transition metals like Fe, Ni, Co, Mn, Cr, V etc., are called DMS (Diluted Magnetic Semiconductors) materials. About 5 – 10 % of these transition elements can be added as dopants in semiconductors like Si, Ge, Sn, SiC, and other III-V and II-VI compound semiconductors. Other examples of DMS materials are Zn1-xMnxSe, Pb1-xMnxTe, Cd1-xMnxTe, MnTe, MnSe etc. There are so many other possible DMS materials such as (Zn, Cd, Hg – O, S, Se, Te), which form the paramagnetic DMS materials, (Zn, Cd, Hg – B, Al, Ga, In), (N, Ps, Sb – O, S, Se, Te), (N, P, As, Sb – B, Al, Ga, In), form ferromagnetic DMS materials. Another set of DMS materials are based on ZnO, i.e., Zn1-xTMxO (TM = Transition Metal) DMS materials, can be utilized for making chips which can store data in terms of the magnetic spins of the dopant atom. Hence both the charge and spin of the electrons can be effectively utilized in the data storage phenomenon.

The DMS materials can be grown as thin films as well. The candidate for thin film growth is Mn / GaAs. This can be achieved either by ion implantation are standard thin film growth techniques. The bulk materials like Ge1-xTMx (TM = Transition Metal) Si1-xTMx, can be grown using high temperature methods.

The growth and study some DMS materials using bulk crystal growth, thin film or Colloidal (Gel) preparation techniques is being attempted. The grown samples are being characterized by X-ray diffraction using single crystal or powder samples and the X-ray structure will be determined. The complete structure of the host and dopant atoms will be studied. Since the systems will be doped ones, it is appropriate to use techniques for studying the local structure of the systems using Pair Distribution Function too, apart from Full profile powder refinement techniques such as Rietveld technique. Other tools like MEM (Maximum Entropy Method) can also be used to study the electronic structure of the DMS materials.

Other characterization technique like measurement of magnetic susceptibility and moment, will also be carried out using standard methods. At least three DMS materials with different (doping) transition metal elements, with different concentrations will be studied in the present work.

The main objectives of the present work can be categorized as follow.,

1. Growth of some DMS materials.
2. X-ray powder and single crystal data collection of the grown materials.
3. Development of the computer programs necessary for the work.
4. Physical characterization, magnetic conductivity etc.
5. Complete structure characterization using Rietveld and single crystal refinement techniques, (Average Structure) Pair Distribution Function (Local Structure), and bonding using Maximum Entropy Method (MEM).

Many novel aspects on the structural, bonding, and physical properties of DMS materials will be analyzed. A clear understanding of the atomic level properties will gained on DMS materials.