Chapter 7 *Conclusion and Future scope*

In the present thesis, we have examined the structure, optical and magnetic properties of $CeCr_{1-x}Fe_xO_3$ ($x = 0 \leq x \leq 0.5$) along with temperature dependent magnetic structure. The important findings of the thesis work are outlined below:

- $CeCr_{1-x}Fe_xO_3$ (x = 0 and 0.05) compounds were synthesized via one step nitrate solution combustion method. Rietveld refinement of XRD patterns revealed that the compounds were stabilized in an orthorhombic distorted perovskite structure with a Pnma space group (no-62). After increasing x to 0.05, we observed an increase in bond length and lattice volume which could be attributed to the difference in ionic radii of Fe^{3+}(0.645 Å) and Cr^{3+}(0.615 Å). Through transmission electron micrographs, we showed the particle size increased from ~45 nm to ~66 nm, band gap decreased from from 2.9 to 2.6 eV when x increased from 0 to 0.05. From magnetization vs. temperature, we observed a reduction in Neel temperature from 260 to 253 K, accompanied by the emergence of new magnetic ordering at 315 K after doping. The magnetic ordering at 315 K could be attributed to AFM ordering of Cr^{3+}-O-Fe^{3+}, whereas decrease in T_N could be ascribed to the decrease in super exchange bond angle Cr(Fe)-O2-Cr(Fe). Additionally, we observed a two-fold increase in T_{comp} and T_{SR} and a new magnetization compensation below T_{SR} after increasing x to 0.05. Such magnetic anomalies were understood based on the interaction between Cr^{3+}, Ce^{3+} and Fe^{3+} moments and their temperature dependent magnetic behavior. For the first time, we demonstrated field induced bipolar magnetization switching below T_{comp} in this

compound. Both of the compounds had a stable bipolar magnetization switching behavior and an optical band gap in the visible range. Hence, these materials hold potential for applications in photo catalysis, spin resolution, and magnetic switching devices.

- With an increase in x from 0.06 to 0.1, structural distortion increased in the orthorhombic Pnma structure with an increase in lattice parameter and lattice volume attributed to the higher ionic radii of Fe^{3+} (0.645Å) compared to Cr^{3+} (0.615Å). The distortion in structure resulted from the tilting of octahedra was further supported by the change in Ag(6) mode of Raman spectra. Magnetization data revealed that with an increase in Fe^{3+} concentration, T_{N1} increased above 390 K and suppressed the Cr ordering temperature T_N to 245 K. With increasing x, the M_{FC} were found to be positive at $x > 0.08$ which could be attributed to domination of external field over the internal field due to Cr^{3+} moment. Apart from this, the decrease in T_{comp} and increase in T_{SR} were also the consequences of higher external field over the internal field. Besides, magnetization reversal with spin reorientation, the bipolar switching behavior was also observed for $x = 0.06$. The presence of bipolar switching behavior emphasizes the potential application in data storage as well as magnetic switching based nonvolatile magnetic memory devices.
- With an increase in Fe concentration (x) from 0.2 to 0.5, structural analysis from Rietveld refinement of the XRD pattern confirmed the single phase orthorhombic distorted perovskite structure with a Pnma space group. With increasing x, the lattice parameter (a, b and c) and volume increased linearly which suggested the incorporation of Fe^{3+}as well as Fe^{2+} at Cr^{3+} site. Elemental analysis confirmed the

formation of Fe^{2+} and Cr^{6+} along with Fe^{3+} and Cr^{3+}, and their formation also increased with increase in *x*. The band gap decreased from 2.48 to 1 eV as *x* increased from 0.2 to 0.5, can be attributed to the increased in the ratio of Fe^{2+}/Fe^{3+} which introduced a trap state in the band gap and reduced its size. Furthermore, the spin reorientation temperatures T_{SR1} and T_{SR2} increased from 62 K to 138 K and 37 K to 83 K, respectively, when *x* increased from 0.2 to 0.5. This increase in T_{SR1} and T_{SR2} was attributed to the enhanced Ce^{3+}-Fe^{3+} and Fe^{3+}-Fe^{3+} magnetic interactions resulting from the substitution of Fe. Coercivity initially increased upto T_{SR1} and then decreased with increasing temperature for all samples. The tuning of the band gap in the visible region, spin reorientation with coercivity, collectively make these materials suitable candidates for multifunctional application.

- We investigated nuclear and magnetic structure along with magnetic properties of $CeCrO_3$ synthesized through one step solution combustion method. Temperature dependent nuclear structure analysis from time of flight neutron diffraction demonstrated no structural changes within the temperature range 6-300 K. Magnetic structure analysis showed possibility of multiple magnetic structure such as Γ_4, Γ_2, and Γ_1 at high and low temperature due to less difference in lattice parameter a and c. Magnetization vs. temperature clearly indicated the transformation of magnetic structure around T_{SR}. The weak Ferromagnetism with small coercivity in MH loop at T_{max} (215K) confirmed the Γ_4 (G_x, A_y, F_z) magnetic structure while increased coercivity below T_{SR} indicated the Γ_2 (F_x, C_y, G_z) type magnetic structure. Therefore, neutron diffraction along with magnetization measurement stablished a

transformation for Γ_4 (G_x, A_y, F_z) to Γ_2 (F_x, C_y, G_z) type spin reorientation in pure $CeCrO_3$.

Future scope

1. In this thesis, we have limited ourselves to structural, optical, and magnetic properties of transition metal Fe doped rare earth orthochromite $CeCr_{1-x}Fe_xO_3$ (x = 0 and 0.5). One can study the effect of rare earth or different transition metals doping in orthochromite on structural, optical, and magnetic properties.
2. Apart from that, it would be interesting to explore the magnetic structure of these compounds using Neutron diffraction.
3. In addition, it would also be interesting to prepare thin films of these compound to study structural, optical, and magnetic properties and their comparative study with the present results.
4. Catalytic activity of these rare earth chromites have not been well studied in the literature. Thus, it is necessary to investigate the catalytic properties. In addition, their applications in hydrogen generation using water splitting remain unexplored.