**INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI**
**SHORT ABSTRACT OF THESIS**

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## SHORT ABSTRACT

A detailed Density Functional theory calculations and experimental studies have been reported on few novel spinel cobaltites. A substantial increase in the size of the unit cell along with the collapse of long-range antiferromagnetic (AFM) ordering with spin-orbit compensation effect among the key features noticed as the octahedral Co site is diluted with non-magnetic cations. The bandstructure calculations from DFT+U were compared with the experimental observations and it was observed that the increase of the size of the dilutants triggers a drastic decrease in the energy band gap. The normal spinel $Co_2RuO_4$ exhibits AFM transition at Néel temperature ($T_N$) ~ 15.2 K, along with a spin-glass state below $T_N$ mainly governed by ordering of the spins of $Co^{2+}$ ions occupying the A-site. We found that the spin-glass phase was mainly originated due to the exchange interaction between the $Co^{2+}$ ions on the A-site and randomly distributed $Ru^{3+}$ on the B-site. We also report a detailed Field-Temperature (H-T) phase diagram of $Co_2RuO_4$ system for different H for $T < T_N$. Further, using the low temperature (1.6K-300K) neutron diffraction technique, a detailed structural, magnetic and spin dynamics of single/poly crystals of $Co_2TiO_4$ and $Co_2SnO_4$ were investigated. Both these compounds exhibit highest magnetic intensity from the $(111)_M$ reflection due to Ferrimagnetic ordering, which sets in below $T_C$ = 48.6 K and 41 K for $Co_2TiO_4$ and $Co_2SnO_4$, respectively. Finally, using the first-principles methods the electronic structure and magnetic properties of Ge diluted $Co_2TiO_4$ spinels ($Co_2Ti_{1-x}Ge_xO_4$) were extensively studied and we proposed a new approach of tailoring Pyrochlore geometry that led to remarkable change in their electronic and magnetic structure by tuning the cationic disorder.