



Beitrag ID: 91

Typ: Talk

## probing structure and magnetism in a2comno6 (a = lu, ho) geometrically frustrated double perovskites

Compounds in Double perovskites (with general formula  $A_2B'B''O_6$ ) are receiving significant attention in recent research work due to their potential applications in variety of fields [1]. These are derived from simple perovskite structure  $ABO_3$  (where A: large electropositive cation and B: small transition metal ion), and possesses diverse chemical and physical properties, ranging from insulating to metallic electronic structures and several magnetic orderings and frustrated states. This versatility originates due to the structural and compositional flexibility of the perovskite framework [2,3]. With the advent of spin frustrated multiferroics, wherein ferroelectricity is driven by exotic magnetic ordering rather than non-centro-symmetric crystal structure, understanding rare earth based double perovskites ( $RE_2B'B''O_6$ ) becomes crucial where partial or complete cation substitution at different degrees at R and B', B'' sites provide more flexibility to tailor physical properties such as it affects exchange pathways, influencing magnetic order, and can induce mixed valence states, modifying electron density and magnetic coupling[4]. Doping also introduces lattice distortions, affecting magnetic anisotropy, and allows precise control over magnetic transitions temperature. Furthermore, controlled substitution can create competing interactions, leading to exotic magnetic states such as spin liquids and multiferroics. Thus, exploring and innovating magnetic materials like A-site doped double perovskites is crucial for advancing material science, as they provide exceptional solutions for efficient, sustainable, and high-performance technologies.

Here we present synthesis and characterisation of  $A_2CoMnO_6$  (A= Lu, Ho) double perovskite by employing ceramic route. Phase formation was confirmed by powder x-ray diffraction (XRD) and phase purity was ascertained by employing room temperature neutron diffraction using PD-III powder diffractometer at Dhruva, BARC India. The phase stability was confirmed by low temperature x-ray diffraction (LT-XRD) ranging from 12 K–300 K) by employing 18kw Rigaku TTRAX III attached with CCR. The figure 1 shows Rietveld [5] fitted x-ray diffractogram, which confirms the compound crystallizes in monoclinic structure with P21/n space group goodness of fitting and cell parameters are exhibited in relevant figures. The structural analysis shows the the system is geometrically frustrated as the evidences of anti site disorder is observed which has strong correlations to the physical properties, especially the magnetic properties. The results of temperature dependent magnetization along with isothermal magnetization shows that with the isovalent doping of partially 4f filled  $Ho^{3+}$  into the fully filled 4f  $Lu^{3+}$  there is an enhancement in curie temperature from 30 K to liquid nitrogen temperature (~80 K). While comparing the structure part Holmium with ionic radius (~1.015 Å), is expected to induce larger lattice distortion compared to Lutetium (0.816 Å) influencing the super exchange interactions between Co and Mn sites, affecting octahedral tilting and magnetic coupling. We are in a process of analysing the temperature dependent neutron diffraction data (2 K-300 K) to understand the magnetic structure as  $Ho^{3+}$  is magnetic ion (10.6  $\mu_B$ ) and  $Lu^{3+}$  is nonmagnetic also the analysis microscopically explore role of antisite disorder in magnetic structure and correlate ferroelectric and structural parameters. Advanced characterizations viz. heat capacity, AC susceptibility and dielectric study are underway to understand magnetic interactions, and electric properties

[1] S. N. Achary, V. Katari, F. N. Sayed and A. K. Tyagi, J. Chem. Sci. 96,131, 2019.

[2] Y. Mao, J. Parsons, J.S. Mcloy, Nanoscale, 5, 04720, 2013.

[3] HS Nair, R. Pradheesh, Yinguo Xiao, et al., J. Appl.Phys., 116, 123907. 2014

[4] A. Harbi, Y. Le Godec et al., Phys. Rev. B., 104, 054404. 2021

[5] J. Rodriguez-Carvajal, Phys. B., 5 192,1993

athiraraghu92@gmail.com , sdkaushik@csr.res.in

**Autoren:** RAGHU, Athira (UGC DAE ConsortiumFor Scientific Research Mumbai Centre India); Dr. KAUSHIK, S.D. (UGC DAE ConsortiumFor Scientific Research Mumbai Centre India)

**Co-Autoren:** Dr. V.B., Jayakrishnan (Bhabha Atomic Research Centre); Dr. HARIKRISHNAN, R. (Indian Institute of Technology Madras)

**Vortragende(r):** RAGHU, Athira (UGC DAE ConsortiumFor Scientific Research Mumbai Centre India)

**Sitzung Einordnung:** Frustrated spin systems

**Track Klassifizierung:** Frustrated spin systems