

Complex magnetic order at the W-Type Hexaferrite $SrCo_2Fe_{16}O_{27}$

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Single phase magnetoelectric multiferroics combine electric and magnetic dipoles offering attractive possibilities for the development of energy efficient miniaturized devices in information and communication technologies. However, despite more than a decade of intensive research, few of them have been identified where both ferroic orders coexist at room-temperature with strong enough magnetoelectric coupling. A step towards this goal is the search for materials where the ferroelectric polarization is magnetically induced. Hexaferrites are complex ferrimagnets where several promising examples have been found, partially due to the possibilities to tune their properties with chemical substitutions. Among them, W-type hexaferrites have been less explored. Introducing Co in this family of ferrites drives the system away from simple uniaxial anisotropy. In the case of $BaCo_2Fe_{16}O_{27}$, a conical distribution of the magnetic easy axis prone to induce ferroelectricity exists, but it vanishes at room temperature [1]. While in $SrCo_2Fe_{16}O_{27}$, emergence of non-collinear magnetic order at room temperature has been reported [2].

In this work we focus on $SrCo_2Fe_{16}O_{27}$. Using density functional theory (DFT) with a Hubbard U correction, we investigate the relative stability of Co substitutions, to provide an accurate map of the relationship between electronic and magnetic features with the Co concentration and distribution. Our results evidence a strong preference for Co^{2+} ions to occupy the 6g octahedral sites, which has consequences on the evolution of the system from half-metallicity to an insulating regime as the Co concentrations increases, while preserving the ferrimagnetic order of the parent W-type hexaferrite. Further, also the magnetic anisotropy evolves from a single magnetic easy axis to a more complex magnetic pattern, compatible with a transverse conical state. All these results are in excellent agreement with soft X-Ray resonant magnetic diffraction (SRXD) measurements of single-crystal $SrCo_2Fe_{16}O_{27}$ over a range of sample orientations and magnetic-field geometries, that demonstrate a transverse conical magnetic order at room temperature. The combined theoretical and experimental effort establishes $SrCo_2Fe_{16}O_{27}$ as a prominent candidate to host room-temperature magnetoelectric effects.

References:

- [1] D. Samaras et al., Journal of magnetism and magnetic materials 79 (1989) pp. 193–201
- [2] M. I. Mørch and M. Christensen, Applied Crystallography 56 (2023) pp. 597– 602

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