Interplay of Magnetism, Structure, and Electronic Properties in the Iron-Based Spin ladder $BaFe_2S_3$

Y.OUBAID [1 2], *V. Balédent* [1] , *P. Fertey*[2], *M.Verseils*[2] *and P. Foury-Leylekian*[1]

[1] Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405, Orsay, France.
[2] Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin BP 48, 91192, Gif-sur-Yvette, France

Recently, a family of quasi-1D Fe-based spin ladders compounds with the formula $BaFe_2X_3$, where X represents a chalcogen (Se or S), exhibit superconducting properties under pressures exceeding 10 GPa, with critical temperatures of approximately 10 K or 26 K, depending on the chalcogen species [1]. However, the intriguing properties of these compounds extend beyond superconductivity. At ambient pressure, they behave as Mott insulators and display exotic structural and magnetic phenomena, including multiferroicity near room temperature. As such, these materials encompass key characteristics of strongly correlated quantum systems.

Building on extensive investigations of $BaFe_2Se_3$, this work presents a comprehensive experimental study of $BaFe_2S_3$. A detailed examination of the structural, magnetic, and electronic properties of $BaFe_2S_3$ as a function of temperature—and to some extent under pressure—was conducted using a multi-technique approach. This included X-ray diffraction, neutron diffraction, and synchrotron-based infrared spectroscopy, performed on both powder and single crystals from the same synthesis batch. These experiments were further complemented by ab initio calculations, enabling the construction of a comprehensive picture of the underlying physics as a function of temperature.

Our study has uncovered novel phases featuring new atomic structures, a previously unreported structural transition (to a polar structure), and demonstrating that $BaFe_2S_3$ hosts a combination of an exotic tilted stripe magnetic order, multiferroicity and small magnetoelasticity [2]. These findings have allowed us to refine existing interpretations and establish critical connections between these fundamental parameters.

In particular, we have significantly revised the interpretation of various experimental observations reported in the literature, substantially enhancing our understanding of magneto-elastic coupling, electronic gap opening, and structural degrees of freedom. This refined perspective provides a new foundation for investigating the behavior of these materials under pressure and elucidating the insulator-to-metal transition, which may ultimately lead to superconductivity.

References

[1] H. Takahashi et al. Nature Materials, (2015)
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