Structure and Magnetism of AgF_2: Trigonal Jahn-Teller effect and Emergent Ferroelasticity

Inés Sánchez-Movellán[1], P. García-Fernández[1], J. A. Aramburu[1], M. Moreno[1]

[1]*Earth Sciences and Condensed Matter Physics Department, University of Cantabria, Santander, Spain*

Since the discovery of high-temperature (high-T_C) superconductivity in 1911, many efforts have been made to observe superconducting states at increasing temperatures. The breakthrough came in 1986, with the discovery of superconductivity in layered copper oxides at about 92 K. In these compounds, superconductivity seems to be driven by three main ingredients: (1) layered crystal structure, (2) distorted CuO_6 complexes and (3) strong antiferromagnetic (AFM) coupling in the Cu layer [1].

Superconductivity in cuprates arises from the strong interaction among d^9 electrons, highly localized in the metal slab. In the last two decades, argentates, in particular AgF_2, have attracted a great deal of attention in the search for non-cuprate systems that could display high-T_C superconductivity [2]. AgF_2 has been presented in the literature as a layered system [3] much like La_2CuO_4. However, the apparent layers in AgF_2 show a buckling in the metal planes. A good starting point for understanding the origin of this possible layered structure is to study its parent phase, that can display a higher symmetry than the observed one [4].

Our findings stress the large differences between AgF_2 and layered compounds such as La_2CuO_4. In fact, our results show that the parent phase of AgF_2 is cubic, devoid of any layering. In this phase, Ag^{2+} ions are placed in trigonal lattice sites, allowing the existence of a Jahn-Teller (JT) effect. The observed orthorhombic structure is a consequence of cooperative distortion driving by a local $E\otimes e$ trigonal JT effect. Although the two out-of-plane bonds are softened after the distortion, covalent bonding and electron hopping in this direction remain strong. Interestingly, the JT distortion breaks the geometrical frustration of the parent phase, giving rise to AFM in AgF_2 planes and, as a result of the multiple minima intrinsic to JT effect, this system displays ferroelasticity, a property tightly related to magnetism in AgF_2 [4].

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