Unusually strong antiferromagnetic superexchange in KAgF₃ perovskite

Superconductivity (SC) is an ability of a solid to conduct electric current without any measurable resistance. High temperature SC (at temperatures exceeding -196 °C *i.e.* boiling temperature of N₂) is limited to oxocuprate (Cu-O) materials. These compounds are layered (two-dimensional) materials containing copper and oxygen, and showing distinct $[CuO_2]$ planes in their crystal structure. To achieve SC these Cu(II) materials must be chemically doped to induce partial Cu(III) or Cu(I) oxidation state. The values of the critical superconducting temperature (T_C) for oxocuprates reach up to -109 °C and thus approach those of the inexpensive dry ice cooling baths (-78 °C). However, the value of $T_{\rm C}$ has not been improved for the last 16 years despite enormously intense research worldwide.

It is generally believed that very strong antiferromagnetic (AFM) interactions present in copper(II) oxides give rise to large enhancement of the T_C values, and dramatic frustration of 2D AFM ordering is achieved already at modest doping levels. The values of magnetic superexchange constants, J, which measure the strength of magnetic interactions for undoped oxocuprates(II), reach -190 meV for Sr₂CuO₃ (a record-holding one-dimensional oxocuprate, Figure 1) and usually fall close to -100 to -150 meV for two-dimensional oxocuprates. However, no other materials with equally strong AFM interactions have been known to date.



Fig. 2. The $[AgF_3^{-}]$ sublattice of **KAgF**₃ perovskite: Ag - gray, F red balls. The 1D infinite (AgF^+) chains propagate along vertical direction giving rise to strong 1D magnetic superexchange.

In their research report Dr Dominik Kurzydłowski and Prof. Wojciech Grochala from the University of Warsaw (Poland) joined by their colleagues from Slovenia (Dr Zoran Mazej, Dr Zvonko Jagličić) and

Belgium (Prof. Yaroslav Filinchuk) describe crystal structure, phase transition and magnetic properties of polymorphic forms $KAg(II)F_3$ (Figure This compound belongs compounds known as fluoroargentates(II). The



Fig. 1. Ranking of the AFM superexchange constants, J (listed as negative of J) for various families of chemical compounds: oxocuprates(II) represented by $Sr_2Cu(II)O_3$, two a 1D material which exhibits record value of of -190 meV, followed by *fluoroargentates(II)* 2). as exemplified by 1D $KAg(II)F_3$ with its J of -97 meV, and leaving all other families of to a larger family of compounds behind (with J of -40 meV or less negative).

researchers were able to show that KAgF₃ exhibits a crystallographic phase transition at -47 °C, and that both perovskite-related polymorphs show unusually strong AFM ordering with J value of -97 meV for the high-temperature form. This value ranks fluoroargentates second only to oxocuprates(II). However, strong AFM superexchange in KAgF₃ holds only in one direction, where the infinite (AgF^{+}) chains propagate.

The challenge now remains to prepare a 2D fluoroargentate(II) material with equally large AFM superexchange constants and achieve chemical doping to generate superconductivity.

The article "Unusually strong 1D antiferromagnetic superexchange in perovskite $KAgF_3$ " will be published in Chemical Communications.