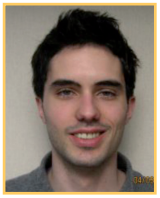

Synthesis and physical properties under high pressure of Cr^{4+}-based compounds

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PHD GRANT

LABORATORY : NEEL

Potential candidates as parent High-Tc compounds are the members of the chromate family, as a result of their layered structure (Fig. 1). Their physics is unknown, due to the harsh high pressure - high temperature synthesis conditions. Several members of the family Æn+1CrnO3n (Æ=Ca, Sr or Ba) were synthesized and studied. New compounds, new crystallographic structures, and new physics were discovered [1]. At n=1, Sr2CrO4 (TN = 112K) showed an unusual anti-Jahn-Teller effect, with an apparently lower symmetry state at low temperatures, explained by the importance of covalency in Cr-O bonds. At n=2, Sr3Cr2O7 (TN = 210K) presented a magnetic and orbital ordering transition, demonstrated by theoretical calculations to be the first evidence of orbital singlets (Fig. 1) [2]. In the previously unknown Ca system, Ca2CrO4 is a central step towards superconductivity, due to its almost metallicity that encourages further pressure and doping studies. At n=3, Ca4Cr3O10, presents another important type of ordering [3], now under theoretical analysis. We are currently working to optimally dope these materials in order to destabilize the antiferromagnetic state and hopefully obtain a metallic and superconducting state.

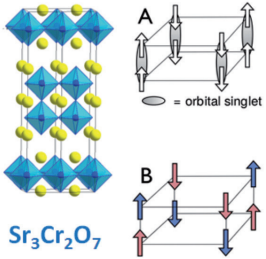

Fig. 1: Left: crystal structure of Sr3Cr2O7 with bilayer of CrO2 planes. Right: Two different orderings of 3d electron spins (arrows) and orbitals (colors) in the bilayer obtained by numerical Lanczos calculations (A) and analytical calculations (B).

OUTCOMES

[1] Ba19Cr12O45 : A high pressure chromate with an original strucutre solved by electron diffraction tomography and powder X-ray diffraction, Inorg. Chem. 56, 6404 (2017).

[2] Singlet orbital ordering in bilayer Sr3Cr2O7, Phy. Rev. Lett. 118, 207207 (2017).

[3] Structural and physical properties of the high pressure perovskite layered Sr4Cr3O10 chromate, J. Solid State Chem. 251, 164 (2017).

Oral presentation: CMD 25 – JMC 14, Paris, France, 2014; 54th EHPRG Meeting, Bayreuth, Germany, 2016.

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