MS24-O2 Spin, charge and momentum densities of YTiO3 perovskyte

Mohamed Souhassou[1], Voufack Bolivard , Nicolas Claiser, Maxime Deutsch, Claude Lacomte, Jean Michel Gillet[2], Pietro Cortona[2], Zeyin Yan[2], Iurii Kibalin[3], Béatrice Gillon[3], Florence Porcher[3], Arsen Gukasov[3], Yoshiharu Sakurai[4], Masayoshi Itou[4], Masahisa Itoh[5]

1. CRM2 Université de Lorraine Nancy France
2. Laboratoire SPMS, CentraleSupelec, Université Paris-Saclay, France
3. Laboratoire Leon Brillouin, CEA/CNRS, France
4. JASRI/ SPring8, Japan
5. Gunma University, Japan

email: Mohamed.Souhassou@univ-lorraine.fr

High resolution X-ray (XRD) and polarized neutron diffractions (PND) are routinely used to model charge and spin densities of localized electrons, while inelastic Compton scattering (ICS) is a valuable mean for determining delocalized electrons. Our objective is to construct a unique electron density model common to these three experimental data sets. We have demonstrated that a joint refinement of a multipolar model based on polarized neutron and X-ray diffraction data is possible and brings more insight in the electron distribution [1]. The inclusion of ICS data implies to go beyond the atom centered model to take into account bicentric terms. As the multipolar model is thus no more adapted, a new model based on atomic orbitals under development will be discussed and applied to a YTiO3 perovskite crystal. This compound is ferromagnetic at low temperature (below 29K), suggesting that a single d electron (0.84mB/mol) mainly localized on the Ti atom gives rise to the magnetic interactions.

Reference 1. "First spin-resolved electron distributions in crystals from combined polarized neutron and X-ray diffraction experiments". Maxime Deutsch, Béatrice Gillon, Nicolas Claiser, Jean-Michel Gillet, Claude Lecomte, and Mohamed Souhassoua,*IUCrJ. 2014 May 1; 1(Pt 3): 194–199.*

Keywords: charge spin densities , xray diffraction, polarised neutron diffraction, magnetic compton scattering, joint refinement, magnetic materials

MS24-O3 New antiferromagnets $[CuX(pyz)_2](BF_4)$ with X = Cl and Br.

Mariusz Kubus[1,2], Arianna Lanza[2], Nicola Casati[3], Piero Macchi[2], Lukas Keller [1], Christoph Fiolka[2], Jürg Schefer[1], Christian Rüegg [1], Karl Krämer[2]

1. Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, CH–5232 Villigen PSI, Switzerland
2. Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3012 Bern, Switzerland
3. Laboratory for Synchrotron Radiation – Condensed Matter, Paul Scherrer Institute, CH–5232 Villigen PSI, Switzerland

email: mariusz.kubus@psi.ch

The structures of new compound $[CuX(pyz)_2](BF_4)$ with $X = Cl^-$ and Br^- and pyz = pyrazine were determined by single crystal X-ray diffraction. These tetragonal compounds crystallize in space group *P4/nbm*. They are built from $[Cu(pyz)_2]^{2+}$ layers which are connected by X^- ions along the *c*-axis. Charge is compensated by BF_4^- ions in the voids of the 3D coordination compound. The antiferromagnetic interactions between the Cu^{2+} ions are mainly two-dimensional (2D) located within the $[Cu(pyz)_2]^{2+}$ layers. This results in a broad maximum of the magnetic susceptibility around 9 K. Towards lower temperature a kink is observed at 4 K which indicates long-range 3D magnetic order. The magnetic unit cell is doubled along the *c*-axis (k = 0,0,1/2) and the ordered magnetic moment amounts to $\mu_x = 0.76(8)\ \mu_B/Cu^{2+}$ at 1.5 K. The moments are antiferromagnetically coupled along the *b*- and *c*-axes. Long-range 3D magnetic order is observed below $T_N = 3.9(1)$ K. A fit of a 2D Heisenberg model to the magnetic susceptibility data results in $J_{||}$ = 9.6 K.

Keywords: 2D antiferromagnet, copper, pyrazine, DMC, XRD, ESR