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Experimental charge and spin densities studies on perovskite of YTiO 3 through Joint refinement of X-ray and polarized neutron diffraction data

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The study and the understanding of both physical and chemical properties of inorganic materials remain a perpetual challenge. In the present work, the modelling of charge densities of both paramagnetic and ferromagnetic perovskite structure of YTiO 3 is undertaken. The structural analysis of this inorganic compound in these two magnetic phases showed that the shape of Ti octahedron is irregular expressing the interactions between electron of Ti atom and O atoms of its environment. The charge density around Ti atom changes significantly between paramagnetic and ferromagnetic phases. The spin-split multipolar model is used in the frame of a joint refinement of X-ray (XRD) and polarization neutron (PND) diffraction data [1] in ferromagnetic phase. The experimental distributions of alpha and beta spin electrons is obtained and their representation agrees with the orbital ordering suggested by previous work of Ito et al. [2] and Hichikawa et al. [3, 4] from X-ray magnetic diffraction (XMD) and PND respectively. Its ferromagnetic order is due to the presence of an unpaired electron localized on Ti atom. The spin density distribution shows the shape of t 2g orbital for the unpaired electron. Furthermore, the provided modelling of charge density shows a charge depletion around Ti atom towards the O atoms described by e g orbitals, meanwhile an accumulation of the density in bisecting directions expresses the t 2g orbitals. Theoretical calculations based on density functional theory (DFT) methods were also carried out and a comparison with these results will be done.
[1] Deutsch M. et al., IUCrJ , 1,194—199, 2014.
[2] Ito M. et al., Journal of Physics and Chemistry of Solids, 65, 1993—1997, 2004.
[3] Ichikawa H. et al., Physica B, 281, 482—484, 2000.
[4] Kibalin I. A. et al., Phys. Rev. B 96, 054426, 2017.

Primary author: VOUFACK, Ariste Bolivard (Université de Lorraine, Vandœuvre-lès-Nancy, France)

Presenter: VOUFACK, Ariste Bolivard (Université de Lorraine, Vandœuvre-lès-Nancy, France)

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