Spin resolved charge density and wave function refinements: the Mollynx/MoPro software

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We are developing in the CRM2 laboratory a new software: Mollynx. As MoPro or XD, Mollynx is derived from Molly (Hansen and Coppens, 1978) but allows to differentiate the electron spins. This new algorithm has been successively applied to paramagnetic coordination compounds (Deutsch et al., 2012, Deutsch et al., 2014) to organic radicals (Voufack et al., 2017) and to small unit cells inorganic crystals (Voufack et al., 2019).

A more general model based on atomic orbitals (Tanaka, 1988; Tanaka, 1993; Bytheway et al., 2001; Schweitzer, 2006), has also been coded in the Mollynx software. This model should allow calculation of properties derived from the atomic wave functions such as covalency, populations of atomic orbitals, energy, optical properties and can in principle describe bonded pair of atoms with orbitals centered on different atoms (two centres orbital products). This model, extended to spin resolved orbitals, has been applied to the $YTiO_3$ perovskite (figure 1, Kibalin et al., 2021) The radial extension, orientation and population of outer atomic orbitals for each atom have been modelled leading to a clear description of the bonding in this crystal .

Thus Mollynx can refine a spin resolved electron density model based on multipolar or on orbital approach. This presentation will describe some of these results and will focus on the experimental spin resolved atomic orbitals model obtained on the $YTiO_3$ including a comparison with a refinement based on theoretical structure factors calculated using density functional theory and the WIEN2k code (Blaha et al., 2020).

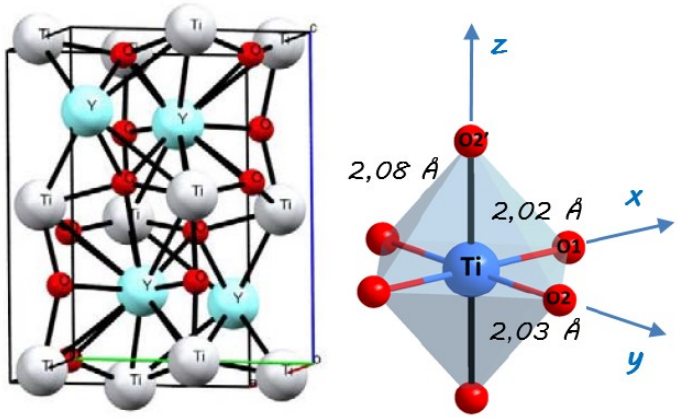

Figure 1: Left : crystal structure of $YTiO_3$ perovskite (space group Pnma), Right: Ti octahedron and local axes

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