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Interplay between H-bonding and charge ordering in $Fe_3(PO_4)_2(OH)_2$ barbosalite

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Charge Ordering (CO) in transition metal oxides is an important parameter for obtaining original magnetic and/or electric properties. That was largely shown within the framework of the studies on colossal magneto-resistance in manganese perovskites and it again seems to be at the origin of the ferroelectricity in $CaMn_7O_{12}$ or $LuFe_2O_4$. The mixed valence of iron in the system is a particular motivation in view of the long lasting research on the understanding of the effects of pressure on charge order/magnetic order in iron compounds such as the $LuFe_2O_4$ new charge ordered state and the pressure dependence of its magnetic order. Here we focus on $Fe^{2+}Fe^{3+}{}_2(PO_4)_2(OH)_2$ barbosalite single crystal, an hydroxyphosphate of iron which exhibits a mixed valence state. High pressure behavior of barbosalite was successfully characterized based on single crystal X-ray diffraction, Raman and infrared spectroscopies. $Fe^{2+}Fe^{3+}{}_2(PO_4)_2(OH)_2$ presents two phase transition at close to 3 and 8 GPa respectively which are clearly governed by an interplay between H-bonding and electron delocalization. Moreover the temperature reaction $Fe^{2+}Fe^{3+}{}_2(PO_4)_2(OH)^{2+}$ $Fe^{3+}{}_3(PO_4)_2(OOH)$.

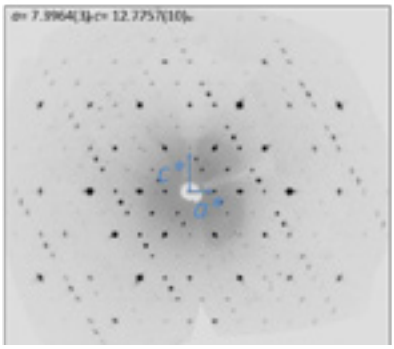

Figure 1: *h0l* reconstruction of the reciprocal space of incommensurate $Fe^{3+}{}_3(PO_4)_2$ (OOH).

Biography

J Rouquette has obtained his PhD in Julien Haines' group in Materials Science (Condensed Matter) from University of Montpellier, France in 2004 and was a Postdoctoral Fellow in Leonid Dubrovinsky's group at the Bayerisches Geoinstitut in Bayreuth University, Germany for two years. He has joined the CNRS as a Researcher in 2004 in the field of ferroelectrics/multiferroics and he defended his Habilitation in 2012 entitled "*insitu* structural studies of ferroic materials as a function of P,T,E,B. He has published more than 50 research papers in these areas.

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