Invited Lecture

Models of polaron fluctuations in $LuFe_2O_4$

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Above its charge ordering temperature of 320 K, $LuFe_2O_4$ becomes disordered with local order indicated by the emergence of diffuse helical scattering in its single crystal x-ray scattering patterns. Here we use 3D-ΔPDF informed Monte Carlo modelling to analyse the diffuse scattering in terms of correlated atomic displacements arising from polarons in the charge-disordered system. The local structure of Lu displacements draws conceptual parallels to the classical models of triangular Ising antiferromagnets with the added complexity of interactions between adjacent Lu planes along the crystallographic [001] direction. Extending the models to include displacements of Fe and O results in an excellent description of the experimental 3D-ΔPDF as shown in Fig. 1 . By analysing the simulated models, we expose aspects of the hidden order of the Fe(II)/Fe(III) valences in the disordered high temperature state of $LuFe_2O_4$. Particularly, we find a strong correlation between the distortion of trigonal bipyramidal coordination and the bond valence sum estimated charges of Fe indicating a Jahn-Teller polaronic character of the charge carriers in the system [1].

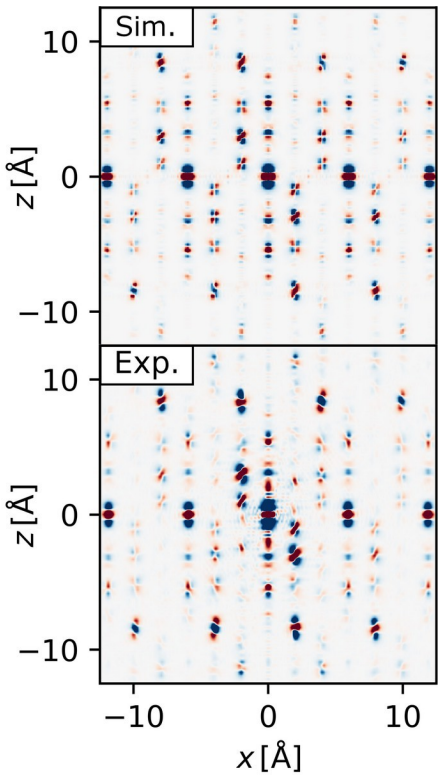

Figure 1. Simulated (top) and experimental (bottom) 3D-ΔPDF of $LuFe_2O_4$ in a representative plane of Patterson space.

[1] Kristoffer A. H. Støckler, Nikolaj Roth, Anders A. Feidenhans'l, Seiya Takahashi, Eiji Nishibori, and Bo B. Iversen, 'Models of polaron fluctuations in $LuFe_2O_4$', *Phys. Rev. Materials*, **8**, 034409, **2024**.