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Pressure induced charge order collapse in Fe₂OBO₃

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Abstract content
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Charge order (CO) refers to the spatial localization of charge carriers on lattice sites with a certain periodicity, resulting in a mixed-valence superstructure within the crystal lattice [1, 2]. Recent work has found evidence of a superstructure in Fe₂OBO₃, with Fe²⁺ and Fe³⁺ valence states close to integer values [3]. This makes Fe₂OBO₃ the archetypal ionic CO compound.

In this study the effect of pressure on the magneto-electronic and structural properties of Fe₂OBO₃ have been investigated by ⁵⁷Fe Mössbauer spectroscopy (MS) and synchrotron x-ray diffraction (XRD) at room temperature [4, 5]. CO is drastically altered at about 11 GPa with a concomitant electron hopping relaxation, Fe²⁺<-> Fe³⁺, as evidenced by MS. Above 16 GPa, the CO has completely 'melted' and electron hopping between distinct Fe sites is dominant. Temperature dependent resistivity measurements up to 22 GPa demonstrate that the electronic structure remains gapped up to this pressure [4].

Analysis of the in-situ XRD data indicates that the ambient pressure P2₁/c monoclinic crystal structure gradually transforms into the high pressure (HP) Pmcn orthorhombic phase, starting at 6 GPa to completion at 22 GPa[4]. Moreover, the unit cell is found to be more compressible along the a-axis (10% over the pressure range up to 30 GPa) compared to the other directions in the unit cell with 3% compressibility over the same pressure range.

The change in volume for the P2₁/c -> Pmcn phase transition is limited to 1% and the bulk moduli of the two structures are quite similar. The CO phase transition at HP was found to be reversible from decompression measurements.

We present our rationalization of the magnetic-electronic ground state of the HP phase where CO is disrupted: MS results, the anisotropic compression and separate resistivity pressure measurements suggest the existence of an 'exotic' dimer Mott insulator phase.

[1] D. Reznik et al., Nature 440, 1170 (2006).

[2] Y.-D. Chuang et al., Science 292, 1509 (2001).

[3] M. Angst et al., PRL 99, 086403 (2007).

[4] G. Diguet et al., PRB 89, 035132(2014).

[5] G. R. Hearne et al. , PRB 86, 195134 (2012).

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