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Metal-insulator transition in $CuIr_2S_4$: XAS results, structure revisited, electronic structure proposed

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Interestingly, the magnetism in the spinel compound Fe_3O_4 (loadstone), constitutes the correlated electron material/problem of the greatest antiquity known to man. The Verwy transition problem in Fe_3O_4 is, by comparison, young at only 67 years of age. Recently experimental and theoretical insights into such exotic magnetic, charge, and orbital orderings in transition metal (T) spinel compounds have been rapidly emerging. The leitmotifs in these works involve: frustrated tripartite crossing 1D chains of edge-sharing T-ligand octahedra; T-d(t_{2g}) orbital ordering onto subsets of these chains which involve d-d overlap; dimmer formation on these chains; and/or charge ordering on the chains dependent on band filling. Understanding the low temperature structural and metal (M) to insulator (I) transition in the spinel compound $CuIr_2S_4$ provides a key link in the generalization to other such systems. S *K*-edge X-ray absorption spectroscopy (XAS) measurements across this M-I transition reflect a dramatic Ir *d*-electronic state redistribution[1]. These results stimulated a detailed re-evaluation of the of *I*-phase crystal structure in terms of: decoupled chains of IrS_6 octahedra along the (110)-type directions; and an Ir^{3+} (Ir^{4+}-Ir^{4+}) Ir^{3+} repeat pattern ordering, where the (Ir^{4+}-Ir^{4+}) pair forms a dimmer. Further, the electronic state changes, evidenced by the XAS, motivated a model in which the I-phase involves: an orbital ordering of the highest lying t_{2g} electron into 1D chains; the 3/4 filling of this 1D band dictating the periodicity of the orbital/charge ordering; and the direct t_{2g}-t_{2g} dimmer bonding production of an antibonding state prominent in the S-K edge spectrum. The generalization of these concepts to other transition metal spinels will be addressed. [1]M. Croft, W. Caliebe, H. Woo, T. A. Tyson, D. Sills, Y. S. Hor, S-W. Cheong, V. Kiryukhin, and S-J. Oh, Phys. Rev. B 67 (Rapid Comm.), 201102 (2003)