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Evidence for non-metallic behaviour in tetragonal - FeS (mackinawite)

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In comparison to its well known isostructural counterparts, FeSe and FeTe, tetragonal FeS (mackinawite) has largely been unexplored in the literature. Despite some recent theoretical papers which have discussed recently the plausibility of mackinawite exhibiting a superconductive state, there is a comparative lack of experimental data on mackinawite. There is, for instance, no reported low temperature resistivity measurements available. This is possibly due to factors such as its sensitity to oxidation, the abscence of a conventional solid-state method for its synthesis and its reported phase transistions to interrelated compounds in the Fe-S system, particuarly Fe_3S_4 (which can commence within a few days of the sample synthesis). We report transport measurements for mackinawite at atmospheric pressure and under hydrostatic pressure and some recent photoelectron spectroscopy results which show that semiconducting-like behaviour is observed. Furthermore, up to the maximum pressures applied, the semiconducting-like behaviour is retained but with a gradual flattening of the resistivity curve, suggesting that the system will eventually undergo a semiconductor – metallic transition with a further application of pressure. Interestingly, this contradicts band structure and more recent density functional theory (DFT) calculations which predict a metallic system. In this presentation we discuss this disagreement between the experimental theoretical data. Focusing on the plausibility of electron correlation in mackinawite. A phenomenon that has already been shown to play a role in tetragonal FeSe and which we believe is a factor fundamental to understanding the observed semiconducting-like behaviour in this complex Fe-S system.