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Investigation into the feasibility of alkali/alkaline earth metal intercalation into the tetragonal - FeS (mackinawite) structure

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Tetragonal FeS (mackinawite), is the third, elusive member of the thoroughly investigated (11) Fe-based superconducting family. A debate has existed in the literature as to whether this compound is either semiconducting or metallic. However, in our recent work we were able to recently show, for the first time experimentally, the low-temperature transport behaviour of mackinawite,[1] and reveal that, in reality, it accommodates a complex interplay of localisation behaviours [2] (Fig 1). Localisation which inhibits its true metallic nature, and instead gives rise to semiconducting-like transport behaviour. Now that we have established this, it is interesting to attempt to intercalate mackinawite with foreign elements such as alkali/alkaline earth metals in attempt to alter this state (i.e. quench the localisation behaviour) and induce superconductivity. This has already proven successful to enhance the T_c of FeSe *via* the intercalation of host materials such as K and Li/amide/ammonia. One particular challenge however is that mackinawite cannot be synthesised using conventional solid-state methods (unlike its iso-structural counterparts FeSe and FeTe) and it quickly begins to degrade above temperatures as low as 30 °C. Therefore solvothermal alternatives must be adapted, such as the recent ammonolysis reactions which have proven so successful for FeSe. The outline of this presentation is to discuss the practicality of applying the same techniques to mackinawite. Is the structure stable during the ammonolysis? Can foreign elements be introduced between the layers e.g. Li, K, Ba. If so, how does this affect their properties? And finally, can a superconducting state be induced?

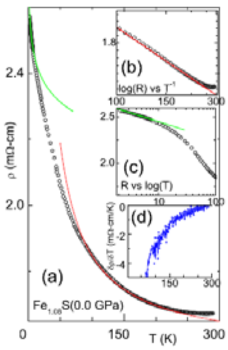

Fig 1 Summary of the transport behaviour of mackinawite, at high-temperature Arrhenius-like band gap behavior is observed whereas at low temperatures Anderson localisation takes over

[1] S. Denholme, S. Demura, H. Okazaki, H. Hara, K .Deguchi, M. Fujioka, T. Ozaki ,T. Yamaguchi, H. Takeya and Y. Takano. *Mater. Chem. Phys.*, **147**, 50, (2014) [2] S. Denholme, H. Okazaki, S. Demura, K .Deguchi, M. Fujioka, T. Yamaguchi, H. Takeya, M. ElMassalami, H. Fujiwara, T. Wakita, T. Yokoya, Y. Takano, *Phys. Rev. B.*, (submitted)