

Abstract Submitted
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Electronic Structure and Magnetic Properties of CsFe₂Sb₂ DAVID

J. SINGH, LIJUN ZHANG¹, ORNL — Iron based arsenide superconductors generally show higher critical temperatures than phosphides, while the antimonides cannot be studied because the corresponding compounds do not form. Within the ThCr₂Si₂ structure, BaFe₂As₂ and BaFe₂P₂ are known compounds, while BaFe₂Sb₂ is not. However, synthesis of CsFe₂Sb₂ was reported by Noack and Schuster in 1994. Here we report density functional studies of the electronic structure and magnetism in this material, as compared to the arsenide, KFe₂As₂. CsFe₂As₂ is found to be an antiferromagnetic metal with interesting similarities to the arsenides.

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