Abstract Submitted
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Double-Exchange physics in Non-Fermi-Liquid FeCrAs PATRICK O'BRIEN, Binghamton University, TURAN BIROL, Rutgers University, SHIVAM GHOSH, Cornell University, MICHAEL LAWLER, Binghamton University, Cornell University, FECRAS COLLABORATION — We focus on the problem of determining the microscopic physics of the bad antiferromagnetic metal FeCrAs[1]. It has been argued to be underscreened Kondo-like[2] due to large spin moments on the Cr atoms. Using LDA+U, we show that indeed Kondo-like physics is likely. In particular, we find the band structure and Fermi surface to be hypersensitive to small changes in the Hund's coupling J with little evidence for crystal field splitting. We then propose a simple three dimensional lattice model using hybrid orbital ideas to capture hopping parameters and a Kondo coupling to capture the limit where J is larger than the crystal field splitting. This model is therefore distinct from one proposed in Ref. [3] which assumes J is less than the crystal field splitting. We chose its parameters based on a best fit to the DFT results and use it to study the stability of the observed $\sqrt{3} \times \sqrt{3}$ magnetic order on the kagome-like Cr lattice as a test of the model. [1] W. Wu et al, 2009 EPL 85 17009 [2] A. Akrap et al, Phys. Rev. B 89, 125115 [3] J.G. Rau and H.Y. Kee, Phys. Rev. B 84, 104448

Patrick O'Brien
Binghamton University

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