Abstract Submitted
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Effects of Doping and Coulomb Correlations on Tc and Competing Phases in Half-metallic Double Perovskites[1] DANIEL KESTNER, ONUR ERTEN, OINAM NGANBA MEETEI, MOHIT RANDERIA, NANDINI TRIVEDI, The Ohio State University — Double perovskites such as Sr_2FeMoO_6 (SFMO) are rare examples of materials with half-metallic ground states and a ferrimagnetic T_c much greater than room temperature. We have shown that the electronic and magnetic properties of SFMO are well described by a generalized double exchange model [1] for itinerant electrons from Mo coupled to localized Fe spins. However, the simplest model proves inadequate when SFMO is electron-doped by La-substitution on the Sr sites. Ignoring Coulomb correlations for the itinerant electrons, the ferromagnetism of Fe spins becomes progressively weaker with electron doping, and eventually the model is unstable to a metallic antiferromagnetic ground state. This is in contradiction with experiments [2], which find a ferromagnetic T_c increasing with carrier concentration and no evidence for an antiferromagnetic state up to $SrLaFeMoO_6$. In this talk we will show that the Hubbard U on the Mo-site is responsible for the observed doping trends. We will show that correlations stabilize the ferromagnetism, with the observed $T_c(n)$ behavior, and that the antiferromagnetic metal is not a competitive state for reasonable values of n.
[1] O. Erten et al, PRL 107, 257201 (2011)
[2] J. Navarro et al, PRB 64, 092411 (2001).

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