

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Theory of magnetic and transport properties of double perovskites¹ OINAM NGANBA MEETEI, ANAMITRA MUKHERJEE, MOHIT RANDEIRA, NANDINI TRIVEDI, PATRICK WOODWARD, The Ohio State University — We map out the finite temperature phase diagram of the generalized double exchange model for double perovskites $A_2BB'O_6$ by self consistently solving the tight-binding Hamiltonian of the “fast” electrons moving in a background of “slowly” fluctuating classical spins. We investigate the stability of ferromagnetic and various antiferromagnetic phases as a function of electron density, the B - B' charge transfer energy, the direct B' - B' hopping and various exchange interactions. We compute the temperature and doping dependence of the B -site magnetization and conduction electron polarization. We also investigate the effects of antisite (B/B') disorder on magnetism and transport. We thus gain insight into material trends in the properties of $A_2FeB'O_6$ and $A_2CrB'O_6$ families, with $B' = Mo, W$ and $A = La, Ca, Sr$.

¹Supported by the NSF-MRSEC grant DMR-0820414

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Date submitted: 20 Nov 2009

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